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Claim (s)

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Abstract

Drawing (s)

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DUPLICATE

INHIBITORS

Field of Invention

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The present invention relates to methods of designing inhibitors of FIH using the crystal structure of FIH, and to inhibitors of FIH and their use in the treatment of ischaemia.

Background of the Invention

In cells of many organisms exposure to an environment in which oxygen is depleted relative to optimal levels induces a hypoxic response. In these hypoxic cells, activation of a transcriptional cascade involving hypoxia inducible factor (HIF) directs a series of adaptive responses that enhance oxygen delivery or limit oxygen demand. Activation of HIF in cancer and ischaemic hypoxic vascular diseases has revealed its important role in human pathology and demonstrated that manipulation of HIF activity has important therapeutic potential.

The HIF transcriptional complex comprises an αβ heterodimer, HIF-β being a constitutive nuclear protein that dimerises with oxygen regulated HIF-α subunits (Semenza, G. L. (2000) Genes Dev. 14, 19831991). The activity of HIF-α, is suppressed by oxygen-dependent modification catalysed by a series of Fe^(II) and 2OG dependent dioxygenases that hydroxylate specific HIF-α residues. In the presence of oxygen in human HIF-1α, 4-hydroxylation of Pro402 or Pro564 by a set of HIF prolyl hydroxylase isozymes (PHD1-3) (Epstein et al. (2001) Cell 107, 4354; Bruick, R. K., and McKnight, S. L. (2001) Science 294, 13371340) mediates its recognition by the von Hippel-Lindau (VHL) ubiquitin ligase complex and consequent targeting for proteasomal destruction (Ivan et al. (2001) Science 292, 464468; Jaakkola et al (2001) Science 292, 468472, WO 02/074981). In a complementary mechanism FIH catalyses β-hydroxylation of HIF-1α Asn803 (Lando et al, (2002) Science 295, 858861) blocking interaction with the transcriptional co-activator p300 (Dames et al., (2002) Proc. Natl. Acad. Sci. U. S. A. 99, 52715276; Freedman et al, (2002) Proc. Natl. Acad. Sci. U. S. A. 99, 53675372). In hypoxia, limitation of enzymatic activity

allows HIF-a to escape destruction and become transcriptionally active.

Inhibition of HIF hydroxylases strongly activates the HIF transcriptional cascade even in the presence of oxygen (Epstein et al.(2001) Cell 107, 4354). Thus, inhibition of the HIF hydroxylases results in a pro-angiogenetic response that may be used in the treatment of cardiovascular diseases/ischaemic hypoxic vascular diseases including myocardial infarction and anaemia. A problem with this approach is that the human cells contain other enzymes belonging to the same family as the HIF hydroxylases, i.e. utilising dioxygen (a cosubstrate), 2-oxoglutarate (20G) (a cosubstrate) and Fe(II) (a cofactor). Such enzymes are exemplified by phytanoyl coenzyme A hydroxylase, procollagen prolyl-4-hydroxylase, procollagen prolyl-3hydroxylase, gamma-butyrobetaine hydroxylase, Alk B (a DNA repair enzyme) and others including predicted 2OG oxygenases identified on the basis of sequence analyses including a sub-family related to FIH (Hewitson et al., J BIOL CHEM 277 (29): 26351-26355, 2002). It is generally agreed that it is desirable that enzyme inhibitors used as pharmaceuticals are selective for their intended target or the targets involved in producing the desired effect. A lack of selectivity can lead to toxic side effects that render particular compounds unsuitable for use in human or animal therapy. One approach to identifying compounds that are selective for the intended target is to undertake structural, mechanistic and other analyses on the intended agents and to use the information gained to aid in the preparation of selective compounds, or more selective compounds (relative to those previously known), for use as pharmaceuticals for use in humans or animals. Here we describe structural and other studies on the HIF hydroxylases that enable the design of selective inhibitors of FIH and related enzymes.

Summary of the Invention

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The present inventors have now identified the site of hydroxylation of asparagine 803 of HIF-1 α by FIH. In addition, the inventors have obtained the crystal structure for FIH including identification of the binding site and residues involved in the interaction of FIH with HIF.

Accordingly, the present invention provides a method of identifying, screening, characterising or designing a chemical entity which mimics or binds to FIH, which method comprises comparing a structural model of FIH with a structural

3 model for said chemical entity, wherein said structural model of FIH is derived from structural factors or structural coordinates determined by subjecting to X-ray diffraction measurements a crystal comprising FIH. The invention also provides for: the use of the structural co-ordinates obtainable by subjecting a 5 crystal comprising FIH to X-ray diffraction measurements and deducing the structural co-ordinates from the diffraction measurements, to identify, screen, characterise, design or modify a chemical entity; a chemical entity identified by a method of the invention, wherein said chemical entity inhibits the asparaginyl hydroxylase activity of FIH; and 10 a chemical entity of the invention for use in a method of treatment. Description of the Figures Figure 1: 20G binding site. Figure 2: binding of Asn-803. 15 Figure 3: conformation of CAD at site 1; and Figure 4: conformation of CAD at site 2. Detailed Description of the Invention The present inventors have identified the position of asparagine 803 that is 20 hydroxylated by FIH. In addition, the inventors have identified the crystal structure of FIH. This structure therefore allows for identification of the amino acid residues involved in binding of FIH to HIF. The identification of the interaction and the structures allows for the 25 characterisation or identification of chemical entities which can bind and in particular which can inhibit FIH. A number of different types of inhibitors can be identified as discussed in more detail below. The inventors have successfully crystallised human FIH. This the first crystallisation of FIH and has enabled determination of the crystal structure. Coordinates from the crystal analysis are set out in Table 3 below. The studies have 30 allowed analysis of the binding of asparagine-803 of HIF and analysis of the conformation of the c-terminal activation domain (CAD) of HIF at the binding sites

to FIH. The present invention provides the use of the structural co-ordinates of FIH to identify, characterise, design or screen chemical entities. The chemical entities of interest are those which bind to FIH and in particular which inhibit the asparaginyl hydroxylase activity of FIH. In addition, chemical entities may be identified, characterised or designed which are modified asparagine hydroxylases.

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Typically, the structural co-ordinates used are obtainable by subjecting a crystal comprising FIH or a fragment thereof to X-ray diffraction measurements and deducing the structural co-ordinates from the diffraction measurements, to identify, screen, characterise, design or modify a chemical entity. The structural co-ordinates indicate the positions of individual atoms within the crystal and give an indication of the space available for adjusting the position of individual atoms when designing a chemical entity.

The crystal subjected to X-ray diffraction methods comprises FIH or a fragment thereof. The FIH may be from any source but is preferably human FIH. The FIH may be a modified form. For example, the FIH may be modified by insertion, deletion, n-terminal or C-terminal addition, or substitution of amino acid by another amino acid. Amino acid substitutions may be conservative substitutions. Typically, when crystallised, a FIH mutant will adopt a similar 3-dimensional structure to that adopted by the corresponding FIH. A mutant may be an inactive FIH.

References to FIH herein refer to FIH and homologues thereof. Amino acid residues are defined with reference to the position in FIH (see e.g. Hewitson et al). The relevant amino acid residues of homologues of FIH are the equivalent amino acid residues, based on for example the best alignment of homologue to FIH.

A FIH may be isolated by any suitable means for use in crystallisation studies. For example, a FIH may be purified using biochemical means from a suitable source. Typically, however, it will convenient to over express FIH in cells and purify FIH from those cells. Thus, a polynucleotide encoding a FIH may be used in the construction of a vector. The FIH may be crystallised according to any method known to those skilled in the art. X-ray diffraction may be carried according to any suitable method. The data collected from X-ray diffraction experiments may be processed to deduce the structural co-ordinates of FIH using any suitable method.

which binds to FIH, or which acts as an inhibitor of asparaginyl hydroxylase activity. Alternatively, the chemical entity may be a modified FIH to alter the activity of a 5 FIH. A chemical entity which binds to or inhibits FIH is any chemical entity capable of forming an association with the FIH. The binding or inhibition may be non-specific, for example, such an entity may also bind to or inhibit other 2OG oxygenases. Alternatively, an agent may be designed or identified which specifically 10 binds to or inhibits asparaginyl hydroxylases. An agent may be designed or identified which is a specific inhibitor of FIH, but not other asparaginyl hydroxylases. The structural co-ordinates of FIH allows a skilled person to predict which amino acids are important in active site formation and which amino acids are important in contacting the substrate. The substrate binding site may be shown as a 2 15 dimensional representation or a 3 dimensional representation produced by physical models or displayed on a computer screen. Such representations can be used to design, identify or screen chemical entities which bind to or inhibit or are predicted to bind to or inhibit FIH. Such representations can also be used to identify modifications of FIH to alter its activity characteristics. 20 Examples of modifications to FIH include modifications to increase the binding of FIH for its substrate, or to alter the substrate the specificity. Alternative modifications include those which alter the activity of FIH, for example, to remove asparaginyl hydroxylase activity. The representations of the structures may be used in other ways. For 25 example, the representations of the FIH active site may be used to model constraints by the putative introduction of covalent bonds between the atoms which come close together when FIH binds to a substrate. Representation of the active site may be used to predict which residues of FIH are likely to be involved in steric hindrance. Such residues may be modified, replaced or deleted to decrease esoteric hindrance in order to increase avidity of the peptide for its substrates. 30 In general, it will be necessary to process the structural co-ordinates obtainable according to the invention in computer-based methods in order to identify

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The invention provides the use of structural co-ordinates to identify,

characterise, design or screen a chemical entity. The chemical entity may be one

or design chemical entities with the desired molecular structure or to identify chemical entities whose structure is complementary to all or part of another chemical entity of interest. Thus, chemical entities which have a structure similar to FIH may be identified or designed. Chemical entities which bind to FIH may be identified or designed. Preferably, such chemical entities bind at the active site of FIH and in general may act as inhibitors of asparaginyl hydroxylase activity.

Such computer-based methods fall into two broad classes: database methods and *de novo* designed methods. In database methods, the chemical entity of interest is compared to all chemical entities present in a database of chemical structures and chemical identities whose structure is in some way similar to the compound of interest identified. The structures in the database are based either on experimental data, generated by NMR or X-ray crystallography, or models of 3 dimensional structures based on 2 dimensional data. In *de novo* design methods, models of chemical entities, for example such are those which might bind to FIH are generated by a computer program using information derived from known structures and/or theoretical rules.

Similarly, the FIH structural coordinates may be used to screen for the expected activity of chemical entities selected, designed or shown to be modulators such as inhibitors of other hydroxylases, for example prolyl hydroxylases. For example the compounds may be screened to assess the likelihood of a prolyl hydroxylase inhibitor additionally inhibiting FIH hydroxylase. Such screening methods may be useful in identifying agents which selectively inhibit HIF prolyl hydroxylase, but not HIF asparaginyl hydroxylase.

Chemical entities designed or selected according to the methods of the invention may be tested and optimised using computational or experimental evaluation. Experimental methods to assay for the activity of asparaginyl hydroxylase are described in more detail below.

Based on the structure of FIH, a number of different types of inhibitors can be identified. These inhibitors are discussed in more detail below.

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The crystallographic asymmetric unit contains one FIH molecule. However, analysis of crystallographic symmetry revealed a dimeric form of FIH, consistent with native gel-electrophoresis analysis. The dimer interface involves the two C-terminal helices of each molecule in an interlocking arrangement predominantly involving hydrophobic interactions. This unusual interface buries a surface area of 3210 Å², large on average by comparison to other dimeric proteins of this size. Inhibitors of dimerisation include those that bind to residues that form the dimerisation interface including residues selected from 330-346, such as Leu-340 and Ile-344. Inhibitors include peptides or peptide mimetics that correspond to all or part of the FIH residues involved in the dimerisation interface.

For example, such inhibitors may comprise a fragment of FIH, for example, including the residues from 340 to 344, preferably, including residues 330 to 346. Such a fragment may typically have 6 or 10 amino acids in length, preferably, up to 15 or 20 amino acids in length. Alternatively, peptide homologues may be used, for example, which comprise a homologue to the residues of 340 to 344 or 330 to 336, including 1, 2 or more substitutions. Additional agents include peptides or peptide mimetics which can be designed based on the crystal structure to interfere with dimerisation.

Inhibitors exploiting metal binding in FIH:

The structural work defines the presence of Fe(II) at the active site of FIH and by implication related HIF hydroxylases. The iron is bound in an almost octahedral manner by the side chains of His199, Asp201 and His279, the 2-oxo and 1-carboxylate groups of 2OG. In the enzyme-substrate complexes there is a vacant position opposite His279 revealing that the enzyme is primed for dioxygen binding. Accommodation of a ligand opposite His279 may require disruption of the hydrogen bond between Asp201 and CAD Asn803 (the iron and Asn803 β-carbon are only ~4.9 Å apart). Subsequent decarboxylation of 2OG presumably yields an iron-oxo species [Fe^(IV)=O <-> Fe^(III)-O·] that effects oxidation at the carbon of Asn-803 in the C-terminal transactivation domain (CAD) of HIF.

Compounds that contain functional groups that bind to iron are useful as inhibitors of FIH. Examples of such compounds include thiols, alcohols, phenols, carbohydrates, hydroxamates, imidazoles and other heterocycles.

Zn^(II) binds to FIH in an identical manner to Fe^(II) (structure 3), consistent with the metal-mediated hypoxic effect being due to displacement of Fe^(II) from the active site of HIF hydroxylases. Since neither Zn(II) nor other metal inhibitors of FIH can replace Fe(II) as a cofactor in catalysis, compounds that preferentially promote the binding of a metal other than iron [such as Zn(II)] at the active site of FIH act as inhibitors.

A further class of inhibitor are non-metallic inhibitors that operate via competing with Fe(II) for binding at the active site. Such inhibitors may bind to any or all of the triad of residues (His-199, Asp-201, His-279), that bind the Fe(II) at the active site of catalytically active FIH.

Inhibitors exploiting the 2OG binding sites

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The FIH:CAD structures with NOG reveal that like 2OG it is ligated to iron in a bidentate manner and imply it is an inhibitor due to decreased susceptibility to attack by an iron bound (su)peroxide intermediate or by hindering binding of dioxygen to the metal.

The structural studies on FIH reveal the binding interactions for the 20G and NOG. The 5-carboxylate of 20G (and the equivalent carboxylate of NOG) forms hydrogen bonds with the side-chains of Lys214, Thr196 and Tyr145; such interactions are unprecedented in other structures of 20G oxygenases. FIH is further unusual in that Lys214 is on the fourth DSBH β -strand whereas previously assigned basic 20G-5-carboxylate binding residues are at the beginning of the eighth DSBH strand.

The structural studies reveal the FIH residues that form the pocket into which 2OG and NOG bind. In addition to the aforementioned these include the side-chains of Ile-281, Leu-186, Leu-188, Phe-207, Thr-196. Knowledge of these interactions enables the design of improved (as measured by binding parameters) and selective inhibitors. Thus, for example an inhibitor binding in the 2OG binding pocket may form hydrophobic interactions with any or all of the side chains of Ile-281, Leu-186

Leu-188, Phe-207, Thr-196. Further it may form electrostatic or hydrogen bonding interactions with the residues involved in binding the 5-carboxylate of 2OG (Lys214, Thr196 and Tyr145).

5 Inhibitors exploiting the peptide substrate binding site There are two binding sites

The ES complex structures unexpectedly reveal two separate binding sites involving CAD₇₉₅₋₈₀₆ (i.e residues 795-806 of the C-terminal transactivation domain of HIF) (Site 1) and CAD₈₁₃₋₈₂₂ of HIF (Site 2) with contact surface areas of 1640 Å² and 1080 Å², respectively. CAD residues in these regions are conserved in all known HIF-1α and HIF-2α sequences. The electron density for site 1 was of good quality, with only the side-chain of Tyr798 poorly defined, while that for site 2 was at a lower level and quality, probably reflecting weaker binding at this site. CAD₈₀₄₋₈₀₆ and presumably also CAD₈₀₇₋₈₁₁, for which density was not observed, do not form direct interactions with FIH. Kinetic analyses employed to investigate the relative importance of Sites 1 and 2, revealed that fragments containing site 1 only are hydroxylated by FIH but less efficiently than those containing both sites demonstrating that both are important in binding and that both may be exploited in inhibition studies.

At Site 1 CAD₇₉₅₋₈₀₃ are bound in a groove and adopt a largely extended conformation linked to FIH by ten hydrogen bonds. Asn803 of CAD is strikingly buried at the active and directly adjacent to the Fe^(II). CAD Asn803 and Ala804 form a tight turn, stabilised by a hydrogen bond between the backbone carbonyl of Val802 and NH of Ala804, which projects the side chain of Asn803 towards the Fe^(II). The side chain of CAD Asn803 is precisely orientated by three hydrogen bonds to enable hydroxylation at the *pro-S* position of the β-carbon consistent with the NMR assignments (see above) The primary amide of CAD Asn803 is sandwiched between FIH residue Tyr102 and the Fe^(II), and forms hydrogen bonds with the side chains of FIH residues Gln239 and Arg238, residues located on the insert to the DSBH motif. Significantly, the substrate and Fe^(II) binding sites are directly linked since the backbone nitrogen of CAD Asn803 also forms a hydrogen bond (~3 Å) with the

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carboxylate oxygen of Asp201 that is not complexed to the iron. Six additional hydrogen bonds stabilise the binding of FIH to CAD₇₉₅₋₈₀₁.

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In contrast with Site 1, Site 2 is located on the FIH surface and involves only two hydrogen bonds. CAD₈₁₆₋₈₂₃ of Site 2 form an α-helix, in exact agreement with the structure of this region in complex with CBP/p300 (Dames et al., (2002) *Proc. Natl. Acad. Sci. U. S. A.* 99, 52715276; Freedman et al, (2002) *Proc. Natl. Acad. Sci. U. S. A.* 99, 53675372). As in that complex, the highly conserved Leu818, Leu819 and Leu822 sit in a hydrophobic pocket on the surface of FIH and form the basis of the binding interaction and so it is not possible for these residues to bind simultaneously to CBP/p300 and FIH.

The extended loop conformation adopted by the CAD residues at Site 1, contrasts with the α-helical conformation adopted by the same residues when complexed with the 1st transcriptional adaptor zinc-binding domain (TAZ1) of CBP/p300(Dames et al.,(2002) *Proc. Natl. Acad. Sci. U. S. A.* 99, 52715276; Freedman et al, (2002) *Proc. Natl. Acad. Sci. U. S. A.* 99, 53675372). The disordered structure observed for the CAD, and other HIF-α residues, when free in solution may thus reflect a requirement to adopt more than one conformation for complex formation with different proteins.

The changes in the conformation of CAD on binding are complemented by changes in FIH revealing an induced fit binding process; Trp296 of FIH undergoes a 50° rotation about C_{beta}-C_{alpha} to accommodate CAD Val802, while both Tyr102 and Tyr103 become more ordered. Further evidence of induced fit comes from the significant differences in resolution between the structures obtained with and without CAD fragments bound reflecting ordering of FIH that occurs on binding (structure 4, for comparison, represents FIH complexed with Fe^(II) and 2OG alone). Interference in the conformational changes involved in the hypoxic response, in particular those involving the CAD region, e.g. by use of small molecules or by gene or protein therapy, may allow manipulation of the hypoxic response to enable pro or antiangiogenetic responses.

Thus, the structural studies define the (i) FIH residues involved in binding the CAD of HIF (ii) conformation of FIH when CAD is bound and (iii) conformation of CAD when bound to FIH. These results are useful in the design of selective

inhibitors of FIH and related enzymes. Features of the FIH binding Sites may be used to mediate tighter binding of inhibitors to FIH or to obtain inhibitors that do not bind tightly to FIH, i.e. avoid inhibition of FIH.

Inhibitors binding at or close to the Site 1 may exploit electrostatic, hydrogen binding and/or hydrophobic interactions with Tyr-102, Asp-104, Lys-106, Asp-201, Glu-202, Gln-147, Gln-239, residues 299-303, His-313, Ala-317, Ile-318, Asn-321,

binding and/or hydrophobic interactions with Tyr-102, Asp-104, Lys-106, Asp-201, Glu-202, Gln-147, Gln-239, residues 299-303, His-313, Ala-317, Ile-318, Asn-321, Lys-324, Arg-238, Trp-296, Asn-321- Lys-324. Inhibitors binding at Site 1 may mimic or partially mimic the turn conformation adopted by CAD when bound at Site 1.

Inhibitors binding at or close to Site 2 may exploit electrostatic, hydrogen binding and/or hydrophobic interactions with residues Thr-149, Leu-150, Asn-151, Asp-152 and residues Val-159, Phe-162, Leu-163, Trp-167, Gln-181, Leu-182, Thr-183, Ser- 184, Asn- 185. Inhibitors binding at Site 2 may mimic or partially mimic the helical conformation adopted by CAD when bound at Site 2.

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It is recognised that inhibitors need not bind to both Sites 1 and 2, although that they may, and that Site 1 is preferred over Site 2.

Residues 801 – 805 of CAD that bind at Site 1, and in particular residues 802-805 form a turn conformation in which the distance of the backbone C=O of 802 to the backbone NH of 804 is ca. 2.8 Å. Including the H-bond formed between the NH of Ala-804 and the carbonyl O of Val-802 of the HIF-1alpha CAD, the turn contains 7 atoms in a pseudo-ring.

Turns are especially amenable to mimicry by analogues useful for enzyme inhibition or receptor binding.

Examples of turn mimics and their modifications can be found in the following reviews: Hanessian et al, TETRAHEDRON 53: 12789-12854 SEP 22 1997; Gillespie et al, BIOPOLYMERS 43: 191-217 1997; and Burgess et al., ACCOUNTS CHEM RES 34: 826-835 2001). Recent examples of primary reports on turns include the following (and references therein) Maier et al, EUR J ORG CHEM: 2686-2689, 2002; Reid et al, J AM CHEM SOC 124: 5673-5683, 2002; Mahadevan et al, J BIOMOL STRUCT DYN 19: 775-788 2002; Eguchi et al, J MED CHEM 45: 1395-1398 2002; De Borggraeve et al, TETRAHEDRON LETT 42: 4453-

4457 2001; Eguchi et al, TETRAHEDRON LETT 42: 1237-1239 2001; Manzoni et al, TETRAHEDRON 57: 249-255 2001; Jiang et al., HELV CHIM ACTA 83: 3097-3112 2000; Derrer et al, J CHEM SOC PERK T 1: 2957-2967 2000; Belvisi et al, EUR J ORG CHEM: 2563-2569 2000; Claridge et al, BIOORG MED CHEM LETT 6: 485-490 1996.

Inhibitors employing a combination of binding sites

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It is well known that enzyme inhibitors competing for binding at more than one substrate or cosubstrate binding site, sometimes termed bisubstrate inhibitors, can be useful. Examples can be found in Wang et al, BIOCHEMISTRY-US: 15676-15683 2001; and Lerner et al, ANGEW CHEM INT EDIT 40, 4040-4041, 2001.

In the case of FIH and other 2OG oxygenases bisubtrate inhibitors may be useful since features of 2OG binding may be present in more than one enzyme whereas the CAD substrate is unique. Thus, inhibitors that bind to both binding sites may show improved selectivity over those that bind to the 2OG binding site only. The structural analyses enable the identification of such bisubtrate inhibitors. The 2OG and CAD binding sites are linked to each other via a 'channel' extending from the 2-oxo group of 2OG (or NOG) to the beta-carbon Asn-803 in the FIH.Fe.2OG/NOG.HIF(CAD) complexes. In the structures this 'channel' either appears empty but may be occupied by water molecules. The distance from the C of the 2-oxo group of 2OG to the beta-C of Asn-803 is ca. 6 Å. The distance from the 3-C of 2OG to the beta-C of Asn-803 is ca. 6.6 Å. The information from the structural analyses enables the identification of bisubstrate inhibitors.

Inhibitors that bind to the 2OG binding site or part thereof and the peptide substrate

Another class of inhibitors bind to the enzyme-substrate complex, i.e. to FIH.Fe(II).HIF(CAD). The structural analyses enable the identification of such inhibitors. As described above 2OG and CAD binding sites are linked to each other via a 'channel' extending from the 2-oxo group of 2OG (or NOG) to the beta-carbon of Asn-803 in the FIH.Fe.2OG/NOG.HIF(CAD) complexes.

Mechanism based inhibitors

Another class of inhibitors is based upon substrate analogues that can undergo part of the catalytic cycle but either stall at an intermediate stage or cause an aberrant reaction resulting in damage or inhibition. The observation that FIH catalyses hydroxylation of Asn-803 at the beta-position together with the structural analyses enables the design of such inhibitors. Such compounds include analogues of the substrates (inhibitors) in which Asn-803 is replaced with an analogue which does not undergo oxidation such as beta-fluoro- asparagine, beta-di-fluoro- asparagine, beta-methyl- asparagine, beta-dimethyl- asparagine derivatives. Alternatively derivatives that undergo oxidation to give an agent that can be oxidised to give an inactivating group such as an epoxide or metal chelating group may prepared (such mechanism based inhibitors are sometimes referred to as suicide inhibitors). In the case of FIH they include alpha-beta-dehydroasparagine and beta-methylene asparagine.

The crystal structure of FIH also allows identification of those residues involved in asparaginyl hydroxylase activity of FIH. The crystal structures may therefore be used to design modified FIH, for example, which has reduced or no asparaginyl hydroxylase activity, for example, by mutation of critical residue within the active site. In the alternative, those residues involved in substrate binding can be identified and modified, for example, to allow the asparaginyl hydroxylase to accept other substrates than HIF. For example, by enlarging or decreasing the asparagine binding pocket. Such modified asparaginyl hydroxylases can then be produced using standard techniques. The expected activity can then be assayed as described in more detail below, for example, to identify whether the hydroxylase activity with respect to HIF has been reduced or removed, or alternatively, to assess the asparaginyl activity or binding in respect to other substrates.

Compounds which have been identified in accordance with the present invention can be further analysed in assays to monitor for activity of the asparagine hydroxylase enzyme directly. Agents which inhibit or reduce HIF asparagine hydroxylase activity reduce hydroxylation of HIF-α and lead to an increase in the interaction with P300 and in particular the CH1 domain and thus transcriptional activation. This in turn will lead to the activation of systemic local defences against hypoxia or ischaemia that may include the promotion of angiogenesis, erythropoesis,

energy metabolism, inflammation, vasomotor function and will also affect apoptotic/proliferative responses.

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We describe below in more detail a number of different assays that may be carried out to assay the activity of modulators of HIF hydroxylase activity or of modified FIH identified in accordance with the present invention and in particular of asparagine hydroxylase activity, or which affect regulation of HIF- α interaction with p300 in a cell and hence which affect HIF mediated activity. Some of these assays utilise HIF polypeptides, and HIF asparagine hydroxylases. Typically, the assays may utilise a human HIF asparagine hydroxylase such as FIH or a fragment or variant of a human HIF asparagine hydroxylase. These components are described in more detail below. Each of these components, where required, may be provided either in purified or unpurified form, for example, as cellular extracts or by purification of the relevant component from such extracts. Alternatively, the relevant component can be expressed using recombinant expression techniques and purified for use in the assay. Alternatively, the components may be expressed recombinantly in a cell for use in cell based assays.

Typically, a polynucleotide encoding the relevant component is provided within an expression vector. Such expression vectors are routinely constructed in the art and may for example involve the use of plasmid DNA and appropriate initiators, promoters, enhancers and other elements, such as for example polyadenylation signals which may be necessary and which are positioned in the correct orientation in order to allow full protein expression. Suitable vectors would be very readily apparent to those of skill in the art, such as those described in more detail herein with reference to the HIF hydroxylases. Promoter sequences may be inducible or constitutive promoters depending on the selected assay format. The promoter may be tissue specific. Examples of promoters and other flanking sequences for use in the expression vectors are described in more detail herein with reference to the HIF hydroxylases of the invention and in particular to the human HIF hydroxylases.

HIF Polypeptides and Peptide Analogues

The assays of the present invention may use a substrate of a HIF asparagine hydroxylase and in particular an asparagine containing substrate of the enzyme. In

particular, such substrates may be used in assays to monitor for the activity of a modulator of HIF asparagine hydroxylase activity. The substrate may be a HIF polypeptide or peptide analogue thereof. Typically, a HIF polypeptide will be used as the substrate.

Any suitable substrate in which an asparagine residue is hydroxylated by a FIH may be used. In preferred embodiments of the invention, such a substrate is a HIF polypeptide such as a HIF- 1α or HIF- 2α subunit protein or fragment of either or peptide analogue of the subunit or fragment. Preferably, the HIF- α peptide conveys an oxygen regulated response. Preferably, the HIF- α peptide has a CAD domain and is capable of oxygen regulated interaction with p300 and downstream transcriptional activation. Preferably, such HIF- α peptides are capable of interacting with the p300 CH1 domain. Preferably, such HIF polypeptides, fragments or peptide analogues incorporate an asparagine residue equivalent to Asn 803 defined with reference to HIF- 1α . The asparagine equivalent to Asn 803 of HIF- 1α may be determined by aligning the HIF variant, fragment or analogue to the sequence of HIF- 1α to obtain the best sequence alignment and identifying thereby the asparagine equivalent to Asn 803 of HIF- 1α .

A HIF polypeptide may be of eukaryotic origin, in particular a human or other mammalian, HIF- α subunit protein or fragment thereof. Alternatively, the polypeptide may be of *C. elegans* origin. In those assays which monitor for hydroxylation of HIF- α through its interaction with p300, the HIF polypeptide has the ability to bind to a wild type full length p300 protein or a fragment thereof comprising the CH1 domain. Preferably, such binding is able, in a hypoxic cellular environment, to activate transcription.

A number of HIF α subunit proteins have been cloned. These include HIF-1 α , the sequence of which is available as Genbank accession number U22431, HIF-2 α , available as Genbank accession number U81984 and HIF-3 α , available as Genbank accession numbers AC007193 and AC079154. These are all human HIF α subunit proteins and all may be used in the invention. HIF- α subunit proteins from other species, including murine HIF-1 α (accession numbers AF003695, U59496 and X95580), rat HIF-1 α (accession number Y09507), murine HIF-2 α (accession

numbers U81983 and D89787) and murine HIF-3 α (accession number AF060194) may also be used in the invention.

One HIF- α protein of particular interest is the *C.elegans* HIF- α subunit protein. The *C.elegans* system may be used in assays of the present invention.

There are a number of common structural features found in the two HIF- α subunit proteins identified to date. Some of these features are identified in O'Rourke et al (1999, J. Biol. Chem., 274; 2060-2071) and may be involved in the transactivation functions of the HIF- α subunit proteins. One or more of these common structural features are preferred features of the HIF polypeptides.

Variants of the above HIF- α subunits may be used, such as synthetic variants which have at least 45% amino acid identity to a naturally occurring HIF- α subunit (particularly to a human HIF- α subunit such as, for example HIF- 1α), preferably at least 50%, 60%, 70%, 80%, 90%, 95% or 98% identity. Such variants may include substitutions or modifications as described above with respect to HIF hydroxylases. Amino acid activity may also be calculated as described above with reference to HIF hydroxylases.

HIF fragments may also include non-peptidyl functionalities and may be optimised for assay purposes such that the level of identity is lowered. Such functionalities may be covalently bound such as sugars or non-covalently bound such as metal ions.

HIF α polypeptides as described herein may be fragments of the HIF- α subunit protein or variants as described above, provided that said fragments retain the ability to interact with a wild-type p300 CH1 domain. When using proteinogenic amino acid residues, such fragments are desirably at least 20, preferably at least 40, 50, 75, 100, 200, 250 or 400 amino acids in size. Desirably, such fragments include asparagine 803.

Cell based assays of the present invention may involve upregulation of an endogenous HIF- α or expression of a HIF- α by recombinant techniques and in particular of HIF- 1α .

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17 The present invention provides an assay method for an agent identified as a modulator of asparagine hydroxylation of hypoxia inducible factor. The method comprises contacting a HIF asparagine hydroxylase and a test substance in the presence of a substrate of the hydroxylase under conditions in which asparagine hydroxylation occurs in the absence of the test substrate and determining asparagine 5 hydroxylation of the substrate. In an alternative assay, HIF asparagine hydroxylase and the test substance are contacted in the presence of the substrate of the hydroxylase under conditions in which hydroxylation does not occur in the absence of the test substrate. Determination of any asparagine hydroxylation is monitored to identify whether the agent actively acts as a promoter of asparagine hydroxylase. 10 FIH has been found to hydroxylate HIF- α at an asparagine residue within the CAD domain. This hydroxylation mediates p300 binding and in particular, reduces p300 binding. Such binding leads to transcriptional activation. This interaction and activation may also be used as the basis for an assay of the invention. Such assays of the present invention may be used to assay the activity of 15 inhibitors of HIF asparagine hydroxylase activity and are thus preferably carried out under conditions under which asparagine hydroxylation would take place in the absence of the test substance. The assays of the invention may also be used to assay the activity of inhibitors which are specific for HIF asparagine hydroxylases and which do not have activity or are less active with other hydroxylases, for example, 20 such as HIF prolyl hydroxylases or other asparagine/aspartamic acid hydroxylases. The assays of the invention may also be used to assay the activity of hydroxylase modulators, such as HIF prolyl hydroxylase inhibitors which are not expected to have activity on FIH based on structural modelling studies, and hence may be used to identify inhibitors which are specific for prolyl hydroxylase. 25 Methods for monitoring modulation The precise format of any of the screening or assay methods of the present invention may be varied by those of skill in the art using routine skill and knowledge. The skilled person is well aware of the need to additionally employ appropriate 30 controlled experiments. The assays of the present invention may involve monitoring for asparagine hydroxylation of a suitable substrate, monitoring for the utilisation of

substrates and co-substrates, monitoring for the production of the expected products between the enzyme and its substrate. Assay methods of the present invention may also involve screening for the direct interaction between components in the system. Alternatively, assays may be carried out which monitor for downstream effects such as binding of HIF by p300 and downstream effects mediated by HIF such as HIF mediated transcription using suitable reporter constructs or by monitoring for the upregulation of genes or alterations in the expression patterns of genes know to be regulated directly or indirectly by HIF.

Various methods for determining hydroxylation are known in the art and are described and exemplified herein. Any suitable method may be used for determining activity of the HIF hydroxylase such as by substrate or co-substrate utilization, product appearance such as peptide hydroxylation or down-stream effects mediated by hydroxylated or non-hydroxylated products.

Assays may be carried out to monitor directly for hydroxylation of the relevant asparagine residue or another position. Alternatively, assays may be carried out to monitor for depletion of co-factors and co-substrates. Alternatively, such assays may monitor the downstream effects of hydroxylation of HIF or indeed inhibition of hydroxylation of HIF, for example, by monitoring the interaction between HIF and p300 or HIF mediated transcription. Alternatively, reporter gene constructs driven by HIF regulated promoters may be used. Assays are also provided for the identification of enhancers of the activity of the HIF asparagine hydroxylase. Such enhancers may be used to reduce HIFα activity.

In one embodiment, a suitable substrate of the HIF asparagine hydroxylase is provided. This may be HIF- α or a fragment thereof which includes a CAD domain or which includes a residue equivalent to Asn 803 of HIF- 1α . The substrate may not be initially hydroxylated at the Asn 803 position. This may be achieved by providing synthetic polypeptide substrates, or by producing HIF- α polypeptides in bacterial cells, insect cells or mammalian cells or in *in vitro* transcription and translation systems. Alternatively, assays may be carried out over a selected time course such that the substrate is produced during the course of the assay, initially in unhydroxylated form.

suitable means. Small polypeptide substrates may be recovered and subject to 5 physical analysis, such as mass spectrometry or chromatography, or to functional analysis, such as the ability to bind to p300 (or displace a reporter molecule from p300). Such methods are known as such in the art and may be practiced using routine skill and knowledge. Determination may be quantitative or qualitative. In 10 both cases, but particularly in the latter, qualitative determination may be carried out in comparison to a suitable control, e.g. a substrate incubated without the potential inhibitor. Inhibitor compounds which are identified in this manner may be recovered and formulated as pharmaceutical compositions. Assays in accordance with the present invention may involve monitoring for 15 the interaction between p300 and HIF. The interaction between HIF and p300 is mediated by hydroxylation of HIF. Transcription and expression of genes known to be upregulated or down regulated by the presence of HIF could be monitored. In particular, upregulation of HIF regulated genes would demonstrate inhibition of asparagine hydroxylation whereas down regulation would suggest enhancement or 20 promotion of asparagine hydroxylation. In alternative embodiments, reporter constructs may be provided in which promoters mediated by HIF are provided operably linked to a reporter gene. Any suitable reporter gene could be used, such as for example enzymes which may then be used in colorometric, fluorometric, fluorescence resonance or spectrometric 25 assays. HIF asparagine hydroxlase is a 20G dependent oxygenase. In the assay methods described herein, typically the HIF asparagine hydroxylase and the substrate of the hydroxylase are contacted in the presence of a co-substrate, such as 2oxoglutarate (20G). The hydroxylase activity of the HIF hydroxylase may be 30 determined by determining the turnover of the co-substrate. This may be achieved by determining the presence and/or amount of reaction products, such as hydroxylated

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together under conditions which, in the absence of inhibitor provide for

hydroxylation of Asn 803, and the effect of the inhibitor may be determined by determining hydroxylation of the substrate. This may be accomplished by any

The substrate, enzyme and potential inhibitor compound may be incubated

substrate or succinic acid. The amount of product may be determined relative to the amount of substrate. Typically, in such embodiments the substrate may be an HIF- α polypeptide and, for example, the product measured may be hydroxylated HIF- α polypeptide.

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Alternatively, the end-point determination may be based on conversion of HIF α or peptide fragments (including synthetic and recombinant peptides) derived from HIF α into detectable products. Peptides may be modified to facilitate the assays so that they can be rapidly carried out and may be suitable for high throughput screening.

For example, reverse phase HPLC (C-18 octadecylsilane column), may be used to separate starting synthetic peptide substrates for HIF hydroxylase from the asparagine hydroxylated products, as the latter have a shorter retention time in the column. Modifications of this assay or alternative assays for HIF hydroxylase activity may employ, for example, mass spectrometric, spectroscopic, and/or fluorescence techniques as are well known in the art (Masimirembwa C. et al Combinatorial Chemistry & High Throughput Screening (2001) 4 (3) 245-263, Owicki J. (2000) J. Biomol. Screen. 5 (5) 297-305, Gershkovich A et al (1996) J. Biochem. & Biophys. Meths. 33 (3) 135-162, Kraaft G. et al (1994) Meths. Enzymol. 241 70-86). Fluorescent techniques may employ versions of the substrate modified in such as way as to carry out or optimise spectroscopic or fluorescence assays.

For example, HIF α polypeptide may be immobilised e.g. on a bead or plate, and hydroxylation of the appropriate residue detected using an antibody or other binding molecule which binds the CAD binding domain of HIF α with a different affinity when an asparagine 803 is hydroxylated from when the residue is not hydroxylated. Such antibodies may be obtained by means of standard techniques which are well known in the art, e.g. using a hydroxylated HIF α peptide.

Binding of a molecule which discriminates between the hydroxylated and non-hydroxylated form of a HIF α polypeptide may be assessed using any technique available to those skilled in the art, which may involve determination of the presence of a suitable label.

Assay methods of the present invention may also take the form of an *in vivo* assay. The *in vivo* assay may be performed in a cell line such as a yeast strain in which the relevant polypeptides or peptides are expressed from one or more vectors introduced into the cell.

In vivo assays

The assays may be carried out using cell based, organ based or whole animal assays conducted *in vivo*. Such assays may utilize the endogenous expression of the HIF hydroxylase nucleotides and/or polypeptides. In other forms of the invention, upregulation of specific endogenous HIF hydroxylases may be achieved by stimulators of the expression thereof. Such stimulators may be growth factors or chemicals that upregulate specific HIF asparagine hydroxylases. In another form of the assay, nucleotide constructs may be introduced into cells or transgenic animals to increase production of one or more specific HIF asparagine hydroxylases.

HIF complexed with p300 activate hypoxia response elements that are found in the promoters and/or enhancers of endogenous genes that are regulated by the said HIF complexes. Such hypoxia response elements may also be isolated and operationally linked to reporter genes so as to assay the activity of the HIF complex through detection and/or quantitation of the reporter gene or its product. Therefore in a further form of the invention the activity of a HIF- α polypeptide that is regulated by HIF asparagine hydroxylase will be assayed by measuring the effects of the HIF complex on the expression of an endogenous gene or reporter gene that is functionally linked to a HIF binding hypoxia response element. Examples of endogenous genes that are regulated in this way are to be found in the role of the aryl hydrocarbon nuclear translocator (ARNT) in hypoxic induction of gene expression, see for example, Studies in ARNT-deficient cells. S.M. Wood, J.M. Gleadle, C.W. Pugh, O. Hankinson, P.J. Ratcliffe. Journal of Biological Chemistry 271 (1996) 15117-15123, and Hypoxia inducible expression of tumor-associated carbonic anyhydrases, C.C. Wykoff, N.J.P. Beasley, K.J. Turner, J. Pastorek, A. Sibtain. G.D. Wilson, H. Turley, K. Talks, P.H. Maxwell, C.W. Pugh, P.J. Ratcliffe, A.L. Harris. Cancer Research 60 (2000) 7075-7083. Examples include but are not limited to glucose transporter isoform 1, phosphoglycerate kinase-1, carbon anhydrase isoform

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9, vascular endothelial growth factor. Each of said genes contains one or hypoxia response elements that may be isolated and operationally linked as single or multiple copies to a reporter gene for the measurement of activity of a HIF-α polypeptide that varies in accordance with the activity of a HIF hydroxylase.

The activity of genes or gene products that are regulated by a HIF- α polypeptide in accordance with the activity of a HIF hydroxylase affects cellular, organ, and animal physiology. Assays that utilise a specific functional response that is regulated in accordance with the activity of a HIF- α polypeptide in accordance with the activity of a HIF hydroxylase may be used. Such responses include the uptake rate of glucose or glucose analogues that are not metabolized, the growth of blood vessels by angiogenesis, the activity of a carbonic anhydrase enzyme. It is recognised that many other responses that operate at a cellular or systemic level are controlled by the activity of a HIF- α polypeptide in accordance with the activity of a HIF hydroxylase and may be utilized as assays of the said HIF hydroxylase activity in further aspects of the invention,

A HIF-α polypeptide that is a substrate for a HIF hydroxylase may be fused to a further polypeptide so as to cause the activity of the said HIF hydroxylase to regulate the activity of the fusion peptide. Accordingly a further form of the invention provides for the assay of the activity of a fusion polypeptide. In the preferred form such a fusion polypeptide may contain the whole of part of a HIF-α polypeptide, particularly including Asn 803, or the CAD domain. The Gal4 DNA binding domain including the amino acids 1-143 together with the Gal binding upstream activating sequence (UAS) is an example of such a transcription factor and cognate DNA response element whose operation can be assayed by those skilled in the art.

Selectivity

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It may also be advantageous to modulate HIF asparagine hydroxylase selectively, as a single target, or in selected hydroxylase groups as well as an entire family. Agents which modulate HIF asparagine hydroxylase activity are therefore preferably specific i.e. they have an increased or enhanced effect on a HIF asparagine hydroxylase relative to other 2OG dependent oxygenases.

Assay methods as described herein may therefore further comprise contacting the test compound with one or more 2OG dependent oxygenases under conditions in which said 2OG dependent oxygenases are normally active and determining activity of said oxygenases. A difference in activity in the presence relative to the absence of test compound is indicative of the test compound modulating the activity of the one or more 2OG dependent oxygenases.

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A test compound which provides increased or enhanced modulation of a HIF asparagine hydroxylase, relative to the one or more 2OG dependent oxygenases shows selectivity or specificity for the HIF hydroxylase.

2OG dependent oxygenases may include for example, clavaminte synthase, Aik B deacetoxycephalosporin C synthase, collagen-prolyl-4-hydroxylase,collagen prolyl-3-hydroxylase, lysyl hydroxylase, aspartyl hydroxylase, phytanoyl coenzyme A hydroxylase or gamma-butyrobetaine hydroxylase. 2OG dependent oxygenases may be mammalian, preferably human polypeptides.

The invention provides for the use of such selective inhibitors of HIF asparagine hydroxylases in the manufacture of a medicament for the treatment of a condition associated with reduced HIF activity.

Therapeutic Applications

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A compound, substance or agent which is found to have the ability to affect the hydroxylase activity of a HIF asparagine hydroxylase, has therapeutic and other potential in a number of contexts. For therapeutic treatment, such a compound may be used in combination with any other active substance, e.g. for anti-tumour therapy another anti-tumour compound or therapy, such as radiotherapy or chemotherapy.

An agent identified using one or more primary screens (e.g. in a cell-free system) as having ability to modulate the HIF α asparagine hydroxylation activity of a HIF hydroxylase may be assessed further using one or more secondary screens. A secondary screen may involve testing for an increase or decrease in the amount of HIF- α or HIF activity, for example as manifest by the level of a HIF target gene or process present in a cell in the presence of the agent relative to the absence of the agent.

A HIF hydroxylase or a HIF polypeptide may be used in therapies which include treatment with full length polypeptides or fragments thereof, or otherwise modified polypeptides (e.g. to enhance stability or ensure targeting, including in conjunction with other active agents such as antibodies. For example, mutation of HIF-1 α to replace Asn 803 with another amino acid residue may prevent hydroxylation and thus promote interaction of HIF- α with p300 and stimulate transcriptional activation.

Generally, an agent, compound or substance which is a modulator according to the present invention is provided in an isolated and/or purified form, i.e. substantially pure. This may include being in a composition where it represents at least about 90% active ingredient, more preferably at least about 95%, more preferably at least about 98%. Any such composition may, however, include inert carrier materials or other pharmaceutically and physiologically acceptable excipients, such as those required for correct delivery, release and/or stabilisation of the active agent. As noted below, a composition according to the present invention may include in addition to an modulator compound as disclosed, one or more other molecules of therapeutic use, such as an anti-tumour agent.

Products obtained by assays of the invention

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The invention further provides compounds obtained or identified by methods of the present invention, and compositions comprising said compounds, such as pharmaceutical compositions wherein the compound is in a mixture with a pharmaceutically acceptable carrier or diluent. The carrier may be liquid, e.g. saline, ethanol, glycerol and mixtures thereof, or solid, e.g. in the form of a tablet, or in a semi-solid form such as a gel formulated as a depot formulation or in a transdermally administerable vehicle, such as a transdermal patch.

The invention further provides a method of treatment which includes administering to a patient an agent which interferes with the hydroxylation of the asparagine target residue of an HIF α polypeptide by a HIF hydroxylase. Such agents may include inhibitors of asparagine hydroxylase activity.

The therapeutic/prophylactic purpose may be related to the treatment of a condition associated with reduced or suboptimal or increased HIF levels or activity,

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or conditions in which have normal HIF levels, but where an modulation in HIF activity such as an increase or decrease in HIF activity is desirable such as:

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- (i) ischaemic conditions, for example organ ischaemia, including coronary, cerebrovascular and peripheral vascular insufficiency. The therapy may be applied in two ways; following declared tissue damage, e.g. myocardial infarction (in order to limit tissue damage), or prophylactically to prevent ischaemia, e.g. promotion of coronary collaterals in the treatment of angina.
- (ii) wound healing and organ regeneration
- (iii) auto-, allo-, and xeno- transplantation.
- 10 (iv) systemic blood pressure
 - (v) cancer; HIF α is commonly up-regulated in tumour cells and has major effects on tumour growth and angiogenesis.
 - (vi) inflammatory disorders.
 - (vii) pulmonary arterial blood pressure, neurodegenerative disease.

Pharmaceutical Compositions

In various further aspects, the present invention thus provides a pharmaceutical composition, medicament, drug or other composition for such a purpose, the composition comprising one or more agents, compounds or substances as described herein, including HIF asparagine hydroxylase inhibitors, the use of such an composition in a method of medical treatment, a method comprising administration of such a composition to a patient, e.g. for treatment(which may include preventative treatment) of a medical condition as described above, use of such an agent compound or substance in the manufacture of a composition, medicament or drug for administration for any such purpose, e.g. for treatment of a condition as described herein, and a method of making a pharmaceutical composition comprising admixing such an agent, compound or substance with a pharmaceutically acceptable excipient, vehicle or carrier, and optionally other ingredients.

In one embodiment the method for providing a pharmaceutical composition may typically comprise:

- (a) identifying an agent by an assay method of the invention; and
- (b) formulating the agent thus identified with a pharmaceutically

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acceptable excipient.

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The pharmaceutical compositions of the invention may comprise an agent, polypeptide, polynucleotide, vector or antibody according to the invention and a pharmaceutically acceptable excipient.

The agent may be used as sole active agent or in combination with one another or with any other active substance, e.g. for anti-tumour therapy another anti-tumour compound or therapy, such as radiotherapy or chemotherapy.

Whatever the agent used in a method of medical treatment of the present invention, administration is preferably in a "prophylactically effective amount" or a "therapeutically effective amount" (as the case may be, although prophylaxis may be considered therapy), this being sufficient to show benefit to the individual. The actual amount administered, and rate and time-course of administration, will depend on the nature and severity of what is being treated. Prescription of treatment, e.g. decisions on dosage etc, is within the responsibility of general practitioners and other medical doctors.

An agent or composition may be administered alone or in combination with other treatments, either simultaneously or sequentially dependent upon the condition to be treated, e.g. as described above.

Pharmaceutical compositions according to the present invention, and for use in accordance with the present invention, may include, in addition to active ingredient, a pharmaceutically acceptable excipient, carrier, buffer, stabiliser or other materials well known to those skilled in the art. In particular they may include a pharmaceutically acceptable excipient. Such materials should be non-toxic and should not interfere with the efficacy of the active ingredient. The precise nature of the carrier or other material will depend on the route of administration, which may be oral, or by injection, e.g. cutaneous, subcutaneous or intravenous.

Pharmaceutical compositions for oral administration may be in tablet, capsule, powder or liquid form. A tablet may include a solid carrier such as gelatin or an adjuvant. Liquid pharmaceutical compositions generally include a liquid carrier such as water, petroleum, animal or vegetable oils, mineral oil or synthetic oil. Physiological saline solution, dextrose or other saccharide solution or glycols such as ethylene glycol, propylene glycol or polyethylene glycol may be included.

Lactated Ringer's Injection. Preservatives, stabilisers, buffers, antioxidants and/or other additives may be included, as required. Liposomes, particularly cationic liposomes, may be used in carrier formulations. Examples of techniques and protocols mentioned above can be found in Remington's Pharmaceutical Sciences, 16th edition, Osol, A. (ed), 1980. 10 The substance or composition may be administered in a localised manner to a particular site or may be delivered in a manner in which it targets particular cells or tissues, for example using intra-arterial stent based delivery. Targeting therapies may be used to deliver the active substance more specifically to certain types of cell, by the use of targeting systems such as antibody 15 or cell specific ligands. Targeting may be desirable for a variety of reasons, for example if the agent is unacceptably toxic, or if it would otherwise require too high a dosage, or if it would not otherwise be able to enter the target cells. In a further embodiment the invention provides for the use of an agent of the invention in the manufacture of a medicament for the treatment of a condition 20 associated with increased or decreased HIF levels or activity. The condition may, for example, be selected from the group consisting of ischaemia, wound healing, auto-. allo-, and xeno- transplantation, systemic high blood pressure, cancer, and inflammatory disorders. 25 Examples Example 1 The position on Asn803 of human HIF-1\alpha that is hydroxylated was identified as described in the following. cDNA sequences encoding FIH-1 were cloned into the 30 pET28a(+) vector (from Novagen) to yield FIH-1 protein with an N-terminal His6tag to facilitate purification. Purification of crude material by nickel affinity

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aqueous solution which is pyrogen-free and has suitable pH, isotonicity and stability.

Those of relevant skill in the art are well able to prepare suitable solutions using, for

of affliction, the active ingredient will be in the form of a parenterally acceptable

example, isotonic vehicles such as Sodium Chloride Injection, Ringer's Injection,

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For intravenous, cutaneous or subcutaneous injection, or injection at the site

chromatography, followed by thrombin cleavage of the His₆ tag, and size exclusion chromatography (Superdex S75) yielded >95% pure protein by SDS-PAGE analysis. Mass spectrometry confirmed the identity of the isolated species. The 19-residue peptide comprising amino acids 788-806 of human HIF-1 α was modified by aerobic incubation with FIH-1 FIH (Hewitson et al., J BIOL CHEM 277 (29): 26351-26355, 2002) in the presence of ascorbate, DTT, catalase, 2-oxoglutarate, and iron(II) for 30 minutes at 37°C. The reaction was quenched by cooling to 4°C and addition of an equal volume of methanol. Precipitate was removed by centrifugation and the supernatant purified by HPLC using a Jupiter C4 column (15cm x 4.6mm). Peptide was eluted using a gradient of acetonitrile in 0.1% trifluoroacetic acid, freeze-dried from the HPLC solvent for amino acid and mass spectrometric analyses. The sample was freeze-dried a second time from D₂O in preparation for NMR analysis.

Catalytic FIH-1 mediated hydroxylation of a synthetic 19 residue peptide corresponding to residues 788-806 of HIF-1 α was confirmed by mass spectrometric analysis of HPLC purified material: Native peptide 19mer [M+2H]²⁺ = 1026.67Da, modified peptide 19mer [M+2H]²⁺ = 1034.61Da, a mass difference of +8Da of the doubly charged ions, corresponding to +16Da in the peptide (oxygen). N-Terminal Edman degradation of the product peptide gave the following sequence: DESGLPQLTSYDCEVxA, where x was not asparagine. The peak from this (16th) cycle of Edman degradation ran to a similar position as the β -hydroxyasparagine standard. Acid hydrolysis of the modified peptide followed by amino acid analysis showed the presence of β -hydroxyaspartic acid only.

Both 1 H and 13 C chemical shift changes between the 19mer peptide substrate and the HPLC purified incubation product were assessed by 2D 1 H- 13 C HSQC experiments. In the substrate a grouping of four β -CH₂ resonances were assigned as belonging to Asp-1, Tyr-11, Asp-12 and Asn-16 according to their 1 H and 13 C shifts (Evans, J. N. S. (1995) Biomolecular NMR Spectroscopy, Oxford University Press, Oxford, UK). In the product it was clear from both the 2D HSQC and the 1D proton spectra that only three of these four resonances are present. Comparison of the two spectra indicates that the signal assigned to the Asn-16 β -carbon (at δ H 2.813 and 2.695ppm and δ C 37.40ppm in the substrate) has disappeared, consistent with

hydroxylation of the asparagine residue at its β-carbon. The resonances due to the two aspartic acid residues had shifted slightly, presumably due to changes in the protonation state, and now occur at a similar ${}^{1}\!H$ chemical shift as the β -protons of the asparagine in the substrate. A difference in the oxidation state of the cysteine between the two samples in unlikely given the near identical chemical shifts for the cysteinyl β-carbon and hydrogens. The change from a double doublet to a single doublet for the β-hydrogen of the hydroxylated residue also rules out any possibility the observed alterations in the NMR spectrum are due to aggregation. Two new resonances have appeared in the product spectrum at δH 4.913 ppm and δC 56.26 ppm and at 8H 4.654 ppm and 8C 72.22 ppm. These resonances correlate with one another in the 2D COSY spectrum and share a ¹H-¹H coupling constant of 2.4 Hz and are therefore assigned as the CH^{α} - CH^{β} of the hydroxylated asparagine. The appearance of these resonances also coincides with the disappearance of the δH 4.706 ppm and δC 51.43 ppm resonances observed in the substrate spectra, which is therefore assigned as the CH^{α} of the parent asparagine prior to modification. Comparison of the CH^{α} - CH^{β} coupling constant of 2.4Hz observed for the hydroxylated Asn-803, with literature values implied the threo isomer is produced.

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In summary of the above `NMR experiments: The HSQC experiments gave direct evidence for hydroxylation occurring at the β -carbon of the target asparagine, with the hydroxylated β -carbon appearing significantly deshielded (at 72.22 ppm) and the adjacent α -carbon deshielded to a lesser extent (at 56.26 ppm) relative to the parent asparagine. Changes of these magnitudes in the ¹³C chemical shifts are inconsistent with hydroxylation of the side-chain nitrogen, but consistent with hydroxylation at the β -carbon. Further, the ¹³C spectrum of free DL-threo- β -hydroxyasparagine (this study), has resonances at 58.63ppm and 73.85ppm corresponding to α - and β -carbons. The product assignment is also consistent with ¹H-NMR chemical shifts of the α - and β -hydrogens in the β -hydroxyaspartyl residues in EGF-like domains which are 4.48ppm and 4.36ppm respectively (with respect to water at 4.75ppm) when calcium is absent (Selander et al, Biochemistry 29, 8111-8118). The analysis of the coupling constant reported here suggests that the threo-isomer is the one formed on hydroxylation of Asn-803 by FIH-1.

Two reports (Dames et al., (2002) Proc. Natl. Acad. Sci. U. S. A. 99, 52715276; Freedman et al, (2002) Proc. Natl. Acad. Sci. U. S. A. 99, 53675372) reveal how βhydroxylation of Asn-803 of HIF-1a would be damaging to complex formation with p300. Although the position of hydroxylation was not identified in either report, both imply that hydroxylation at the pro-S position of the β -carbon, i.e. to give the threo (2S, 3S)-isomer, would interfere with the hydrogen bonding that maintains the α helical conformation adopted by this part of HIF-1a, and also create a need for the energetically unfavourable desolvation of the hydroxyl group. A steric clash between the inserted pro-S hydroxyl group and Ile-353 (numbering from Dames et a l(2002) Proc. Natl. Acad. Sci. U. S. A. 99, 52715276) of p300 would disrupt the interaction of the two proteins. Presumably the same mechanism is also used to abrogate the interaction of HIF-2 α and p300. The discovery that it is the beta-position of Asn-803 that is modified and the associated mechanistic implications may be used in the design of compounds that bind to p300 thereby displacing HIF-alpha and/in the design of inhibitors of FIH (see below); in both cases to enable pro-angiogenetic pharmaceutical agents.

Example 2

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To obtain an FIH:CAD complex suitable for X-ray analysis without oxidation of the CAD or the Fe^(II), FIH and various CAD fragments from seven to fifty-two residues were co-crystallised with Fe^(II) and 2OG under anaerobic conditions. Structures were also obtained for FIH complexed with Fe^(II) and N-oxaloylglycine (NOG, an FIH inhibitor), (anaerobically) and Zn^(II) and NOG (aerobically). These structures were solved by molecular replacement using a model obtained by multiple anomalous dispersion on selenomethionine-substituted apo-FIH. Crystalline FIH:CAD complexes were obtained with CAD₇₈₆₋₈₂₆, Fe^(II) and NOG or 2OG (structures 1 and 2, Table 1), CAD₇₇₅₋₈₂₆ with Zn^(II) and NOG (structure 3). Crystallisation attempts with CAD₇₈₇₋₈₀₆, CAD₈₅₀₋₈₆₂ (HIF-2α, equivalent to HIF-1α CAD₈₀₂₋₈₁₄) and CAD₈₀₀₋₈₀₆ did not result in FIH:CAD complexes; solution analyses indicated that CAD fragments shorter than twenty resides are not efficient *in vitro* substrates.

Table 1 Summary of FIH:CAD-fragment complex structures

					-			•
PDB ID.				1H2K	1H2L	1H2M	1H2N .	
Rfree (%) R.m.s.d.	from	Struct. 1	(Å)	1	0.149	0.136	0.226	
Rfrec (%)				21.3	21.7	22.5	25.7	
Site 2	CAD	residue	resolved	812-823	813-822 21.7	795-806 813-822 22.5	ı	
Site 1	CAD	residues	resolved	795-806 812-823	795-806	795-806		
Co-crystallisation	CAD peptide			HIF-1α 786-826	HIF-1α 786-826	HIF-1α 775-826	HIF-2α 850-862	
ප්	substrate			NOG	20G	NOG	20G	
Metal				Fe	Fe	Zn	Fe	
Structure Resolution Metal	(Å)			2.15	2.25	2.50	2.84	
Structure	No.			-	2	3	4	_

*Crystalline FIH:CAD complexes were also obtained with Fe $^{(II)}$, HIF-1 α 775-786 and 20G or NOG.

Methods employed in structural work

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Protein expression, purification and crystallisation

FIH, CAD₇₇₅₋₈₂₆ and CAD₇₈₆₋₈₂₆ were prepared as described (Hewitson et al., J BIOL CHEM 277 (29): 26351-26355, 2002). Selenomethionine (SeMet) substituted 5 FIH was produced using a metabolic inhibition protocol and LeMaster media supplemented with 50 mg/l L-selenomethionine. SeMet incorporation was >95 % by ESI-MS. Aerobic crystallisation of SeMet FIH (at 11 mg ml⁻¹) was accomplished by hanging-drop vapour diffusion at 17 °C. The mother liquor consisted of 1.2 M ammonium sulphate, 4 % PEG 400 and 0.1 M Hepes pH 7.5. Crystallisation of FIH:Fe:CAD fragment complexes was accomplished under an anaerobic atmosphere of argon in a Belle Technology glove box (0.3-0.4 ppm O₂) using the same mother liquor and a solution containing FIH (at 11 mg ml⁻¹), Fe²⁺ (1 mM), 2OG/NOG (2 mM) and CAD fragment (1 mM). Crystallisation of FIH:Zn:CAD fragment was accomplished aerobically under similar conditions. Peptides were either synthesised by solid phase peptide synthesis or purchased from Biopeptide Co. (San Diego, USA).

Crystallographic data collection and structure refinement

Crystals were cryocooled by plunging into liquid nitrogen and X-ray data were collected at 100 K using a nitrogen stream. Cryoprotection was accomplished by sequential transfer into a solution containing 1.2 M ammonium sulphate, 3 % PEG 400, 0.1 M Hepes pH 7.5 and 10 % followed by 24 % glycerol. A threewavelength multiple anomalous dispersion (MAD) dataset was collected to 2.9 Å resolution on beamline 14.2 of the Synchrotron Radiation Source, Daresbury, U.K. Data from crystals of FIH:CAD complexes were collected on beamlines 14.2, 9.6 or 9.5 using ADSC Quantum 4 (14.2 and 9.6) or MarCCD detectors (9.5). All data was processed with the program MOSFLM and the CCP4 suite[Collaborative Computational Project Number 4 Acta Crystallogr. D50, 760-763 (1994)]. The crystals belonged to space group P4₁2₁2. Six selenium positions were located and phases calculated using the program SOLVE (Terwilliger et al. D55, 849-861, 1999). Density modification, which increased the figure of merit from 0.56 to 0.66, was performed using RESOLVE (Terwilliger Acta Crystallogr. D56, 965-972 2000).

An initial model was built using the program O (Jones et al, Acta Crystallogr. A47, 110-119, 1991) and refined against the SeMet data (remote wavelength) using the program CNS (Brunger Acta Crystallogr. D54, 905-921, 1998). One cycle of simulated annealing followed by grouped B-factor refinement brought the $R_{\rm free}$ to 36.2 %. Following further rebuilding and refinement, which brought the $R_{\rm free}$ to 32.3 %, the model was transferred to the 2.15 Å dataset. Rebuilding and refinement using REFMAC5 including addition of Fe, substrate and solvent molecules, and refinement of TLS parameters brought the conventional R-factor to 17.8 % and the $R_{\rm free}$ to 21.3 %. The following residues are missing in the current model: 1-15 and 304-306 of FIH, 786-794, 807-811 and 824-826 of the CAD fragment. According to PROCHECK there are no Ramachandran outliers and 90.7 % of residues have most favourable backbone conformations. For the CAD peptide, 77.8% of residues are in the most favourable region with the remaining 22.2 % in additionally allowed regions.

Other structures were solved by molecular replacement using the coordinates from the 2.15 Å data and refinement using REFMAC5. In all structures electron density for the Fe and 2OG/NOG was visible throughout refinement. Significant positive difference electron density was observed between the iron and the CAD Asn803 β-carbon. Since B-factor differences between FIH and CAD imply that the CAD is not at 100 % occupancy, this may represent an alternative binding-mode for the 1-carboxylate 2OG in the absence of substrate although it could also be due to a ligating water molecule, again in the absence of substrate.

Overview of FIH structure

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The core of FIH comprises a double-stranded beta-helix (DSBH or jellyroll) motif formed from eight β -strands, $\beta 8$ - $\beta 11$ and $\beta 14$ - $\beta 17$. Residues 220-259 form an insert between strands 4 and 5 of the DSBH. The bottom face of the DSBH is flanked by an additional four β -strands from the N-terminal region to form an eight-membered antiparallel β -sheet. The N-terminal strand $\beta 1$ bisects the face of the DSBH opposite to the active site. The $\beta 1$ strand has a 360° twist located at a PXXP sequence, in between its interactions with $\beta 14$ and $\beta 2$. A similarly positioned β -

strand is found in most 2OG oxygenases, though not always from the same region of the protein. The sheet-helix-sheet motif formed by β1, α1 and β2 is conserved in all enzymes of this class except proline 3-hydroxylase and a similar fold in this region is found in the related Cu^(II) utilising quercetin 2,3-dioxygenase (QD) (Fusetti et al, STRUCTURE 10 (2): 259-268 2002). The topology of FIH unequivocally defines it as an iron-binding member of the cupin structural family which already includes QD and Mn^(II) utilising Type II phosphomannose isomerase (Clissold, P. M., and Ponting, C. P. (2001) *Trends Biochem. Sci.* 26, 79).

10 Related enzymes to FIH

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FIH has significant sequence similarity with the JmjC homology region of the jumonji transcription factors (Clissold, P. M., and Ponting, C. P. (2001) *Trends Biochem. Sci.* 26, 79; Hewitson et al., J BIOL CHEM 277 (29): 26351-26355, 2002). These proteins are members of the cupin structural superfamily and have been implicated in cell growth and heart development. The 2OG oxygenase iron binding residues had been identified in some JmjC domains but not assigned as an iron binding motif. Sequence searches in the light of the FIH structure reveal many JmjC proteins with conserved residues that include both this motif and others, including FIH residues Lys214 and Thr196 that are unusually involved in binding the 5-carboxylate of 2OG. The structure thus reveals that FIH is a one of a large family of iron and 2OG dependent oxygenases involved in the regulation of transcription. Since some of the assigned JmjC domains other than FIH are associated with diseases and particular phenotypes their (e.g.) inhibition may be of therapeutic value. (See e.g. Hu et al, ONCOGENE 20 (47): 6946-6954 OCT 18 2001 and Clissold, P. M., and Ponting, C. P. (2001) *Trends Biochem. Sci.* 26, 79 and references therein).

Table 2. Partial sequence alignment of FIH with a selection of JmjC domain containing proteins. FIH secondary structure is indicated above the alignment.

Selected 2OG binding residues found in FIH are indicated by dark triangles under the alignment and the two iron binding residues by light triangles. SWALL accession numbers are indicated on the left of the alignment.

Dm Q9VJ97 Sp 013977				Hs 094877	Dm Q9V6L0	Ce Q9GYI4	Rn Q9R153 1	Sc P40034	Dm Q9VНН9	Ce Q20367	Ce Q9BI67	radonas	от бамомз	Dm Q9VU77	Hs Q969Q7	
							PASS1								FIH	
FASDWLNEQLIQQ5KDDYRFVYMBPKNIWISYHADVFGSF6WSTNIVGLKKWLIMPPG FADDWLNAYVIDCESDDFRFAYIGSHLWIGGLHIDVYASHSF8VNLCGVKCWLFIDPK	TILDLVEKESGITIEGYNTP!	TILULUTI I INYG'INALITT	Ì	TVLDVVEEECGISIEGVNTP	TILDYVNKDYNIQİDGVNTA	FEDDLEHYADDKKRPPHRI	-KTDVFQEVM-WSDFGFPGRNGQESTLHT SIGAH PCHLDSYGCNLVFQVQGRKRWHLFPPE	-QNDIVDKIWSFNGHLEKV (11) PKVTK!	eivroidwydvyweko (16) prvorycimsvkncyjdehidfggtsvwyhiirgs (1) kyfwlippt	revodismakrimsdv (11) pxieqicaaaman@y@deffvdeggisvyehverge (4) kieyiaapy	rfvqeismvnriwedv (20) pkveqecia@magbyddegssvyyhiikgekifyiaapt	KIVRKLSWVENLWBEEC (4) PNVQKYCLMSVRDWYMDEHIDFGGTSVWYHVLKGEKIFYLIRPI	AlkedisIpdycti (5) pgavdikami@pag@vgphHydpkhVilcqvegskriilaapa	ELAADLRVSDLDFAQQ(4)-PPDAVNFWISDERAVISMIKDPY	FINNNHINKQQGKRGWGQLTSNLLLIGMEGNVTPAHYDEQ-	· Heart and and control of the contr
EVXT SETT	XTAX E MINK	NINKSTATI	XXX HAVY	ATAR HANK	XTX HE WINK	WEVMPARE	TLWINGLIGH	YILMSVKDA	YCLMSVKNC	ICAAAMAN	FCLA MAG	YCLMSVRD	KAMIJEAG	NEWLEDERA	TITIMEGN	β8
TIGLATOVYAS	PYLYE HAWKES EMWHENDLYSINYNMENTY O	aylyennküseamhtedmdlysinythegap	TERMEDAL TO I	———PYLYT例MWK世生AWHTEDMDLYSINYLHEGEP	AYLYEEMWKITEAWHTEDMDLYSINYMWEITYAA	-rwfvmparsgralhinplgisamysilogh-	ндесильств-	YTOFHLDEAGI	TDEHIDEGI	LEBERT TRANSPORTER	YEDF HVDFGGS	Y DE HIDEGE	NACKHWASA	WISMHKDRY	MENHYDEQ	ρ <u>9</u>
FSWSTNIVGLX	ASIMATHEGEEK	YSINTHEGAP	X SINFLHEGAP	YSINYLHFGEPF	YSINTHEGAPK	SAWKSLLQGHF	CNILVEQVQGR	SVYYNVISGQ	SVWYHILRGS(1)	Svyfhvfkge (4)}	SVYYHILKGE	SVWYHVLKGE	HULLCOVIES	ENVYCVISGHKDFVLIEPH	QNFFAQIKGYKRCILFPPD	β10 310
CMLEIDER	TAKAS YMS X	KIWYALPPA	HOSTATWYN	?KSWYAIPPE	THEVE	KRWVLIPPI	CRWHLEPPE	KRLTLEPRI	CAEMITEL	(IFY LAAPT	TEXTANET .	TEYLIRPT	RILLAAPA	COFVLIPPH	RCILEPPD	β11 ***********************************

Hs = Homo sapiens

Dm = Drosophila melanogaster

Ce = Caenorhabditis elegans

Sc = Saccharomyces cerevisiae.

Rn = Rattus norvegicus

Sp = Schizosaccharomyces pombe

FIH = factor Inhibiting HIF
PASS1 = Protein associating with
small stress protein

TABLE 2

TABLE 3 - Coordinates for structures 1 to 4

Structure 1

```
Below are the coordinates for structure 1 (the 2.15 Å structure of FIH:Fe(II):NOG:CAD):
```

```
HEADER
          TRANSCRIPTION ACTIVATOR/INHIBITOR
                                                   12-AUG-02
                                                                1H2K
          FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX WITH HIF-1 ALPHA
TITLE
TITLE
         2 FRAGMENT PEPTIDE
         MOL ID: 1;
COMPND
         2 MOLECULE: FACTOR INHIBITING HIF1;
COMPND
COMPND
         3 CHAIN: A;
COMPND
         4 ENGINEERED: YES;
COMPND
         5 MOL ID: 2;
COMPND
         6 MOLECULE: HYPOXIA-INDUCIBLE FACTOR 1 ALPHA;
COMPND
         7 SYNONYM: HIF-1 ALPHA, ARNT INTERACTING PROTEIN,
           MEMBER OF PAS PROTEIN 1;
COMPND
COMPND
         9 CHAIN: S;
COMPND 10 FRAGMENT: C-TERMINAL TRANSACTIVATION DOMAIN FRAGMENT
COMPND · 11 RESIDUES 786-826
SOURCE
         MOL ID: 1;
SOURCE
         2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE
         3 ORGANISM_COMMON: HUMAN;
SOURCE
         4 EXPRESSION SYSTEM: ESCHERICHIA COLI;
SOURCE
         5 EXPRESSION SYSTEM STRAIN: BL21(DE3);
SOURCE
         6 EXPRESSION SYSTEM PLASMID: PET28A(+);
SOURCE
         7 MOL ID: 2;
SOURCE
        8 ORGANISM SCIENTIFIC: HOMO SAPIENS;
SOURCE
         9 ORGANISM COMMON: HUMAN;
SOURCE 10 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE 11 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE 12 EXPRESSION SYSTEM PLASMID: PGEX-GP-1
KEYWDS
         FIH, HIF, DSBH, OXYGENASE, TRANSCRIPTION, HYPOXIA,
KEYWDS
         2 2-OXOGLUTARATE, ASPARAGINYL HYDROXYLASE, PHOSPHORYLATION
EXPDTA
          X-RAY DIFFRACTION
AUTHOR
          J.M. ELKINS, K.S. HEWITSON, L.A. MCNEILL, I. SCHLEMMINGER,
AUTHOR
         2 J.F.SEIBEL, C.J. SCHOFIELD
REVDAT
             03-SEP-02 1H2K
JRNL
                    J.M. ELKINS, K.S. HEWITSON, L.A. MCNEILL,
JRNL
            AUTH 2 I.SCHLEMMINGER, J.F. SEIBEL, C.J. SCHOFIELD
JRNL
             TITL
                    FIH: HIF-FRAGMENT COMPLEXES
JRNL
            REF
                    TO BE PUBLISHED
JRNL
            REFN
REMARK
REMARK
         2 RESOLUTION. 2.15 ANGSTROMS.
REMARK
         3 REFINEMENT.
REMARK
         3
REMARK
             PROGRAM
                          : REFMAC 5.0
         3
REMARK
              AUTHORS
                          : MURSHUDOV, VAGIN, DODSON
REMARK
         3
REMARK
         3
               REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK
          3
REMARK
             DATA USED IN REFINEMENT.
REMARK
              RESOLUTION RANGE HIGH (ANGSTROMS) :
                                                     2.15
REMARK
              RESOLUTION RANGE LOW
                                     (ANGSTROMS): 18.50
REMARK
          3
             DATA CUTOFF
                                      (SIGMA(F)) : NONE
                                             (용) :
REMARK
          3
              COMPLETENESS FOR RANGE
                                                    99.28
REMARK
              NUMBER OF REFLECTIONS
                                                     28171
REMARK
          3
```

```
FIT TO DATA USED IN REFINEMENT.
REMARK
         3
              CROSS-VALIDATION METHOD
                                                   : THROUGHOUT
              FREE R VALUE TEST SET SELECTION : RANDOM
REMARK
         3
                        (WORKING + TEST SET) : 0.18026
REMARK
         3
              R VALUE
   ARK
          3
              R VALUE
                           (WORKING SET) : 0.17761
                                                  : 0.21305
  ARK
          3
              FREE R VALUE
REMARK
              FREE R VALUE TEST SET SIZE
         3
                                               (%): 7.7
REMARK
         3
              FREE R VALUE TEST SET COUNT
                                              : 2340
REMARK
         3
REMARK
         3 FIT IN THE HIGHEST RESOLUTION BIN.
              TOTAL NUMBER OF BINS USED
REMARK
          3
                                                             . 20
              BIN RESOLUTION RANGE HIGH
BIN RESOLUTION RANGE LOW
REMARK
          3
                                                           2.150
                                                           2.205
REMARK
          3
REMARK
          3
              REFLECTION IN BIN (WORKING SET) :
REMARK
              BIN R VALUE
          3
                                       (WORKING SET) :
              BIN FREE R VALUE SET COUNT :
REMARK
          3
REMARK
              BIN FREE R VALUE
          3
REMARK
          3
          3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK
REMARK
          3 PROTEIN ATOMS : 2875
REMARK
              NUCLEIC ACID ATOMS
                                         : 0
          3 HETEROGEN ATOMS : 21
REMARK
REMARK
          3 SOLVENT ATOMS
REMARK
          3
REMARK
          3 B VALUES.
         3 FROM WILSON PLOT (A**2): NULL
REMARK
          3 MEAN B VALUE (OVERALL, A**2) : 25.725
REMARK
REMARK
          3 OVERALL ANISOTROPIC B VALUE.
REMARK 3 B11 (A**2): -0.27
              B22 (A**2) :
                                 -0.27
REMARK 3
REMARK 3
              B33 (A**2) :
                                 0.55
              B12 (A**2) :
REMARK 3
                                  0.00
REMARK 3
              B13 (A**2) :
                                   0.00
REMARK 3
               B23 (A**2) :
                                  0.00
REMARK 3
REMARK
          3 ESTIMATED OVERALL COORDINATE ERROR.
REMARK
          3 ESU BASED ON R VALUE
                                                                    (A): 0.174
          3 ESU BASED ON FREE R VALUE
REMARK
                                                                    (A): 0.156
          3 ESU BASED ON MAXIMUM LIKELIHOOD
REMARK
                                                                    (A): 0.147
REMARK
          3 ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2): 5.588
REMARK
          3 CORRELATION COEFFICIENTS.
REMARK
REMARK
          3 CORRELATION COEFFICIENT FO-FC : 0.961
REMARK
              CORRELATION COEFFICIENT FO-FC FREE: 0.947
REMARK
          3
          3 RMS DEVIATIONS FROM IDEAL VALUES COUNT
REMARK
                                                                RMS
                                                                        WEIGHT
REMARK
              BOND LENGTHS REFINED (A): 2973; 0.012; 0.021
              BOND LENGTHS OTHERS .
REMARK
                                            (A): 2561; 0.001; 0.020
              BOND ANGLES REFINED (DEGREES): 4044; 1.374; 1.949
BOND ANGLES OTHERS (DEGREES): 5979; 0.722; 3.000
REMARK
REMARK
              TORSION ANGLES, PERIOD 1 (DEGREES): 352; 4.018; 3.000
REMARK
          3
REMARK
          3
              TORSION ANGLES, PERIOD 3 (DEGREES): 515;17.698;15.000
REMARK
          3
              CHIRAL-CENTER RESTRAINTS (A**3): 416; 0.086; 0.200
              GENERAL PLANES REFINED (A): 3333; 0.005; 0.020
GENERAL PLANES OTHERS (A): 604; 0.002; 0.020
REMARK
          3
REMARK
          3
                                                  (A): 604; 0.002; 0.020

      GENERAL PLANES OTHERS
      (A):
      004; 0.002; 0.002

      NON-BONDED CONTACTS REFINED
      (A):
      714; 0.218; 0.300

      NON-BONDED CONTACTS OTHERS
      (A):
      2499; 0.204; 0.300

      H-BOND (X...Y) REFINED
      (A):
      259; 0.152; 0.500

      H-BOND (X...Y) OTHERS
      (A):
      4; 0.087; 0.500

      SYMMETRY VDW REFINED
      (A):
      18; 0.245; 0.300

      SYMMETRY VDW OTHERS
      (A):
      72; 0.248; 0.300

REMARK
          3
REMARK 3
REMARK 3
REMARK 3
REMARK 3
REMARK
```

```
REMARK
           SYMMETRY H-BOND REFINED
                                        (A): 13; 0.255; 0.500
        3
REMARK
           SYMMETRY H-BOND OTHERS
                                         (A):
                                                1 ; 0.052 ; 0.500
        3
REMARK
        3
        3 ISOTROPIC THERMAL FACTOR RESTRAINTS COUNT RMS
REMARK
                                                           WEIGHT
REMARK 3 MAIN-CHAIN BOND REFINED (A**2): 1777; 0.618; 1.500
                                    (A**2): 2862 ; 1.177 ; 2.000
        3
          MAIN-CHAIN ANGLE REFINED
REMARK
        3 SIDE-CHAIN BOND REFINED (A**2): 1196; 1.812; 3.000
REMARK
          SIDE-CHAIN ANGLE REFINED (A**2): 1182; 3.002; 4.500
REMARK
REMARK 3
        3 NCS RESTRAINTS STATISTICS
REMARK
REMARK
        3 NUMBER OF NCS GROUPS : NULL
REMARK
        3 TLS DETAILS
REMARK
REMARK
        3 NUMBER OF TLS GROUPS :
REMARK
REMARK
        3 TLS GROUP:
                           1
REMARK
        3 NUMBER OF COMPONENTS GROUP:
REMARK
        3
            COMPONENTS
                        C SSSEQI TO C SSSEQI
           RESIDUE RANGE :
REMARK
        3
                             A 15
                                           A 451
            RESIDUE RANGE : S
REMARK
                                 795
                                           S
                                               823
        3
            ORIGIN FOR THE GROUP (A): 21.6620 27.4620 28.2370
        3
REMARK
            T TENSOR
REMARK
        3
                     0.1474 T22:
             T11:
                                  0.0149
REMARK
        3
              T33:
                     0.0919 T12:
                                 -0.0099
REMARK
        3
                    -0.0455 T23:
              T13:
REMARK
        3
                                  0.0363
            L TENSOR
REMARK
        3
                     1.0098 L22:
                                  2.2577
REMARK
        3
             L11:
                     1.2037 L12:
REMARK
        3
              L33:
                                   0.6963
                     0.4840 L23:
REMARK
        3
              L13:
                                  1.0420
REMARK
        3
            S TENSOR
REMARK
        3
               S11:
                     0.0288 S12: -0.1525 S13: -0.0400
        3
                     0.1459 S22:
                                 0.0002 S23:
REMARK
               S21:
                                               0.1021
REMARK
        3
               S31:
                     0.1876 S32: -0.0468 S33: -0.0290
REMARK
        3
REMARK 3 BULK SOLVENT MODELLING.
           METHOD USED : BABINET MODEL WITH MASK
REMARK 3
REMARK 3
           PARAMETERS FOR MASK CALCULATION
REMARK 3
            VDW PROBE RADIUS
                             :
                                  1.40
REMARK 3
            ION PROBE RADIUS
                                  0.80
                             :
REMARK 3
            SHRINKAGE RADIUS
                                  0.80
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS: HYDROGENS HAVE BEEN ADDED IN THE
REMARK 3
           RIDING POSITIONS
REMARK
REMARK
       4 1H2K COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY EBI ON 12-AUG-2002.
REMARK 100 THE EBI ID CODE IS EBI-11170.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE
                                        : X-RAY DIFFRACTION
           DATE OF DATA COLLECTION : 15-MAY-2002
REMARK 200
                              (KELVIN) : 100
REMARK 200
           TEMPERATURE
REMARK 200
           PH
                                         : 7.5
REMARK 200
           NUMBER OF CRYSTALS USED
                                        : 1
REMARK 200
REMARK 200
                                   (Y/N) : Y
           SYNCHROTRON
REMARK 200
           RADIATION SOURCE
                                         : SRS BEAMLINE PX9.6
                                        : PX9.6
REMARK 200
           BEAMLINE
                                        : NULL
 REMARK 200
           X-RAY GENERATOR MODEL
 REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
```

```
REMARK 200 WAVELENGTH OR RANGE
                                      (A) : 0.87
REMARK 200 MONOCHROMATOR
                                           : NULL
REMARK 200 OPTICS
                                            : NULL
REMARK 200
REMARK 200 DETECTOR TYPE
                                           : CCD
REMARK 200 DETECTOR MANUFACTURER
                                            : ADSC
REMARK, 200
            INTENSITY-INTEGRATION SOFTWARE: MOSFLM
REMARK 200 DATA SCALING SOFTWARE
                                           : SCALA
REMARK 200
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 30574
REMARK 200 RESOLUTION RANGE HIGH (A): 2.15
                                       (A): 18.17
REMARK 200 RESOLUTION RANGE LOW
REMARK 200
            REJECTION CRITERIA (SIGMA(I)) : NONE
REMARK 200
REMARK 200 OVERALL.
REMARK 200 COMPLETENESS FOR RANGE
                                      (%): 99.2
REMARK 200
            DATA REDUNDANCY
                                           : 6.3
REMARK 200
            R MERGE
                                        (I) : 0.052
REMARK 200 R SYM
                                        (I) : NULL
REMARK 200
            <I/SIGMA(I)> FOR THE DATA SET : 9.9
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.15
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A): 2.27
REMARK 200 COMPLETENESS FOR SHELL (%): 96.0
REMARK 200 DATA REDUNDANCY IN SHELL
                                      : 3.4
(I) : 0.331
REMARK 200 R MERGE FOR SHELL
REMARK 200 R SYM FOR SHELL
                                       (I) : NULL
REMARK 200
            <I/SIGMA(I)> FOR SHELL
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MAD
REMARK 200 SOFTWARE USED: SOLVE
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS (%): 63
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 3.4
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: 1.2M AMMONIUM SULPHATE, 4% PEG400,
REMARK 280 0.1M HEPES PH7.5, ARGON ATMOSPHERE, 11MG/ML PROTEIN WITH
REMARK 280 1MM FE(II), 2.5MM NOG AND 2.5MM PEPTIDE
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 41 21 2
REMARK 290
REMARK 290
                SYMOP
                       SYMMETRY
REMARK 290
              NNNMMM OPERATOR
REMARK 290
               1555
                        X,Y,Z
                 2555 -X, -Y, 1/2+Z
REMARK 290
              3555 1/2-Y,1/2+X,1/4+Z
4555 1/2+Y,1/2-X,3/4+Z
5555 1/2-X,1/2+Y,1/4-Z
6555 1/2+X,1/2-Y,3/4-Z
REMARK 290
REMARK 290
REMARK 290
REMARK 290
REMARK 290
                7555
                        Y, X, -Z
REMARK 290
                .8555
                       -Y, -X, 1/2-Z
REMARK 290
               WHERE NNN -> OPERATOR NUMBER
REMARK 290
REMARK 290
                     MMM -> TRANSLATION VECTOR
```

```
EMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
                     1 1.000000 0.000000 0.0000000
                                                            0.00000
            SMTRY1
REMARK 290
                       0.000000 1.000000 0.000000
                                                            0.00000
            SMTRY2
REMARK 290
                                                            0.00000
                     1 0.000000 0.000000 1.000000
            SMTRY3
REMARK 290
                     2 -1.000000 0.000000 0.000000
                                                            0.00000
REMARK 290
            SMTRY1
                     2 0.000000 -1.000000 0.000000
                                                            0.00000
REMARK 290
            SMTRY2
                     2 0.000000 0.000000 1.000000
                                                           73.32800
REMARK 290
            SMTRY3
                     3 0.000000 -1.000000 0.000000
                                                           43.08050
            SMTRY1
REMARK 290
                                                          43.08050
                                 0.000000 0.000000
                     3 1.000000
REMARK 290
             SMTRY2
                                                          36.66400
                     3 0.000000 0.000000
                                           1.000000
REMARK 290
            SMTRY3
                                                          43.08050
                                           0.000000
REMARK 290
            SMTRY1
                     4 0.000000
                                  1.000000
                                                           43.08050
             SMTRY2
                      4 -1.000000
                                  0.000000
                                            0.000000
REMARK 290
                                                       . 109.99200
REMARK 290
             SMTRY3
                      4 0.000000
                                  0.000000
                                            1.000000
                                                          43.08050
                                            0.000000
REMARK 290
             SMTRY1
                      5 -1.000000
                                   0.000000
                                  1.000000 0.000000
                                                           43.08050
             SMTRY2
                      5 0.000000
REMARK 290
                                                          36.66400
                      5 0.000000
                                   0.000000 -1.000000
REMARK 290
             SMTRY3
                                                          43.08050
                      6 1.000000
                                  0.000000 0.000000
REMARK 290
             SMTRY1
                      6 0.000000 -1.000000 0.000000
                                                          43.08050
             SMTRY2
REMARK 290
                                                         109.99200
             SMTRY3
                      6 0.000000
                                   0.000000 -1.000000
REMARK 290
                                   1.000000 0.000000
                                                            0.00000
                      7 0.000000
REMARK 290
             SMTRY1
                                   0.000000 0.000000
                                                             0.00000
                      7 1.000000
REMARK 290
             SMTRY2
                      7 0.000000 0.000000 -1.000000
                                                            0.00000
REMARK 290
             SMTRY3
                      8 0.000000 -1.000000 0.000000
                                                            0.00000
REMARK 290
             SMTRY1
                                   0.000000 0.000000
                                                            0.00000
                      8 -1.000000
REMARK 290
             SMTRY2
                     8 0.000000 0.000000 -1.000000
                                                          73.32800
             SMTRY3
REMARK 290
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
                             2 CHAIN(S). SEE REMARK 350 FOR
REMARK 300 WHICH CONSISTS OF
REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
REMARK 300
 REMARK 300 QUATERNARY STRUCTURE FOR THIS ENTRY: TETRAMERIC
 REMARK 300
 REMARK 300 THE PROTEIN IS A HOMODIMER FORMED BY CHAIN A.
 REMARK 300 A HETERODIMERIC ASSOCIATION OF CHAIN A WITH CHAIN S
 REMARK 300 PRODUCES A TETRAMER.
 REMARK 300
 REMARK 300 THE BURIED SURFACE AREA SHOWN BELOW IS AN AVERAGE
 REMARK 300 CALCULATED FOR THE HETEROTETRAMER AND DOES NOT
 REMARK 300 CORRESPOND TO THE BURIED SURFACE AREA FOR THE
 REMARK 300 HOMODIMER OF CHAIN A
 REMARK 300
 REMARK 300 THE HETERO-ASSEMBLY DESCRIBED BY REMARK 350 APPEARS
 REMARK 300 TO BE A CASE OF STRONG CRYSTAL PACKING WITH
 REMARK 300 THE MEAN DIFFERENCE IN ACCESSIBLE SURFACE AREA PER
 REMARK 300 CHAIN BETWEEN THE ISOLATED CHAIN AND THAT FOR
                                           2203.4 ANGSTROM**2
 REMARK 300 THE CHAIN IN THE COMPLEX IS
 REMARK 350
 REMARK 350 GENERATING THE BIOMOLECULE
 REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
 REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
 REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
 REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND
 REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
 REMARK 350
```

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REMARK 350 BIOMOLECULE:
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, S
                      1 1.000000
                                              0.000000
                                                                0.00000
REMARK 350
             BIOMT1
                                   0.000000
REMARK 350
             BIOMT2
                      1
                         0.000000
                                    1.000000
                                              0.000000
                                                                0.00000
REMARK 350
             BIOMT3
                      1 . 0.000000 0.000000
                                               1.000000
                                                                0.00000
             BIOMT1
                      2 0.000000 -1.000000
REMARK 350
                                              0.000000
                                                               86.16100
             BIOMT2
                       2 -1.000000 0.000000 0.000000
                                                               86.16100
REMARK 350
REMARK 350
             BIOMT3
                       2 0.000000 0.000000 -1.000000
                                                               73.32800
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
REMARK 465
             M RES C SSSEQI
REMARK 465
               MET A
                          1
REMARK 465
               ALA A
                          2
                          3
REMARK 465
               ALA A
REMARK 465
               THR A
                          4
REMARK 465
               ALA A
                          5
REMARK 465
               ALA A
                          6
REMARK 465
               GLU A
                          7
REMARK 465
               ALA A
                          8
REMARK 465
                VAL A
                          9
REMARK 465
               ALA A
                         10
REMARK 465
                SER A
                         11
REMARK 465
                GLY A
                         12
REMARK 465
                SER A
                         13
REMARK 465
               GLY A
                         14
REMARK 465
                LYS A
                        304
REMARK 465
                ARG A
                        305
REMARK 465
                ILE A
                        306
REMARK 465
                SER S
                        786
REMARK 465
                MET S
                        787
REMARK 465
                ASP S
                        788
REMARK 465
                GLU S
                        789
REMARK 465
                SER S
                        790
REMARK 465
                GLY S
                        791
REMARK 465
                LEU S
                        792
REMARK 465
                PRO S
                        793
                GLN S
REMARK 465
                        794
REMARK 465
                GLN S
                        807
REMARK 465
                GLY S
                        808
REMARK 465
                SER S
                        809
REMARK 465
                ARG S
                        810
REMARK 465
                ASN S
                        811
REMARK 465
                GLN S
                        824
REMARK 465
                VAL S
                        825 -
                ASN S
REMARK 465
                         826
REMARK 470
REMARK 470 MISSING ATOM
REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;
REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;
REMARK 470 I=INSERTION CODE):
REMARK 470
              M RES CSSEOI
                            ATOMS
REMARK 470
                GLU A 15
                              CG
                                   CD
                                        OE1
                                             OE2
REMARK 470
                GLU A 29
                              CG
                                   CD
                                        OE1
                                              OE2
REMARK 470
                ASN A 87
                              CG
                                   OD1
                                        ND2
                LYS A 106
REMARK 470
                              CD
                                   CE
                                        ΝZ
 REMARK 470
                LYS A 115
                              CG
                                         CE
                                              NZ
                                   CD
REMARK 470
                ARG A 117
                              CG
                                   CD
                                        NE
                                              CZ
                                                        NH2
                                                   NH1
```

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GLN A 133
GLN A 136
REMARK 470
                            CG
                                 CD
                                      OE1
                                           NE2
REMARK 470
                            CG
                                 CD
                                      OE1
                                           NE2
             GLN A 137
                            CG
                                 CD
                                      OE1
                                           NE2
REMARK 470
              ARG A 156
                            CG
REMARK 470
                                 CD
                                      NE
                                            CZ
                                                 NH1
                                                      NH2
REMARK 470
              LYS A 157
                            CD
                                 CE
                                      N2.
REMARK 470
              LYS A 311
                                      CE
                                            NZ
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 3(1X, A4, 2X), 12X, F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500 M RES CSSEQI ATM1 ATM2 ATM3
                                             ANGL. DEV. = 9.3 DEGREES
REMARK 500
              ASN A 84
                          N
                               - CA - C
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD AND BY MORE THAN 0.150 ANGSTROMS (M=MODEL
REMARK 500 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
REMARK 500 NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 1X, 2 (A4, A1, 3X), 12X, F5.3)
REMARK 500
REMARK 500 EXPECTED VALUESS: ENGH AND HUBER, 1991
REMARK 500
REMARK 500
            M RES CSSEQI ATM1
                                 RES CSSEQI ATM2
                                                  DEVIATION
REMARK 500
              MET A 343 SD
                                 MET A 343 CE
                                                   -0.249
 REMARK 500
 REMARK 500 REMARK: NULL
 REMARK 500
 REMARK 500 GEOMETRY AND STEREOCHEMISTRY
 REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
 REMARK 500
 REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
 REMARK 500
             ATM1 RES C SSEQI
 REMARK 500
                                  ATM2 RES C SSEQI
                                                                DISTANCE
 REMARK 500
 REMARK 500
                           209
                                   0
                                                 108
                                                                   2.20
              0
                   GLN A
                                        HOH Z
 REMARK 525
 REMARK 525 SOLVENT
 REMARK 525
 REMARK 525 THE SOLVENT MOLECULES ARE GIVEN CHAIN IDENTIFIERS TO
 REMARK 525 INDICATE THE PROTEIN CHAIN TO WHICH THEY ARE MOST CLOSELY
 REMARK 525 ASSOCIATED WITH:
 REMARK 525
              PROTEIN CHAIN SOLVENT CHAIN
 REMARK 525
                Α
                                Z
 REMARK 525
                                Н
```

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REMARK 525
REMARK 525 THE FOLLOWING SOLVENT MOLECULES LIE FARTHER THAN EXPECTED
REMARK 525 FROM THE PROTEIN OR NUCLEIC ACID MOLECULE AND MAY BE
REMARK 525 ASSOCIATED WITH A SYMMETRY RELATED MOLECULE (M=MODEL
REMARK 525 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
REMARK 525 NUMBER; I=INSERTION CODE):
REMARK 525
REMARK 525 THESE MOLECULES CAN BE PLACED WITHIN 5.00 ANGSTROM OF THE
REMARK 525 OBSERVED OLIGOMER BY APPLYING THE SYMMETRY TRANSFORMATION
REMARK 525 INDICATED.
REMARK 525
                           ORIGINAL COORDINATES
REMARK 525 M RES CSSEQI
                                                  SYMMETRY TRANS.
                                                                      DIST.
REMARK 525
                            X Y Z
                         12.359 41.757 15.368
REMARK 525 1 HOH W 531
                                                   005
                                                             545
                                                                      2.38
REMARK 525 · 1 HOH W 609
                          10.971 45.216 18.991
                                                   005
                                                            545
                                                                      3.25
REMARK 525 1 HOH W 576
                          42.075 52.163 47.994
                                                            665
                                                    008
                                                                      2.28
                                                            555
REMARK 525 1 HOH W 687
                          28.879 5.577 12.106
                                                    005
                                                                      2.82
                          24.396 12.792 8.360
                                                            555
REMARK 525 1 HOH W 674
                                                    005
                                                                      3.20
                        27.797 7.170 2...
26.874 53.406 28.524
                                                            555
REMARK 525 1 HOH W 543
                                                    005
                                                                      2.83
REMARK 525 ·1·HOH W 607
                                                          . 665
                                                    800
                                                                      2.97
REMARK 600
REMARK 600 HETEROGEN
REMARK 600
REMARK 600 FOR METAL ATOM FE
                              FE2 A1350 THE COORDINATION ANGLES ARE:
REMARK 600 1 HIS
                  199A NE2
REMARK 600 2 ASP
                    201A OD2
                                   104.0
REMARK 600 3 HIS
                                   85.8 88.0
163.5 92.4 96.8
                    279A NE2
REMARK 600 4 OGA 1351A O2
REMARK 600 5 OGA 1351A 02'
                                   86.4 168.8 97.0 77.1
REMARK 600
                                            2
REMARK 700
REMARK 700 SHEET
REMARK 700 THE SHEET STRUCTURE OF THIS MOLECULE IS BIFURCATED. IN
REMARK 700 ORDER TO REPRESENT THIS FEATURE IN THE SHEET RECORDS BELOW,
REMARK 700 TWO SHEETS ARE DEFINED.
REMARK 800
REMARK 800 SITE
REMARK 800 SITE_IDENTIFIER: FE1
REMARK 800 SITE DESCRIPTION: FE BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE_IDENTIFIER: OGA
REMARK 800 SITE DESCRIPTION: OGA BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE IDENTIFIER: SO1
REMARK 800 SITE DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE IDENTIFIER: SO2
REMARK 800 SITE DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 1D7G
                              RELATED DB: PDB
REMARK 900 A MODEL FOR THE COMPLEX BETWEEN THE
REMARK 900 HYPOXIA-INDUCIBLE FACTOR-1 (HIF-1) AND ITS
REMARK 900
            CONSENSUS DEOXYRIBONUCLEIC ACID SEQUENCE
REMARK 900 RELATED ID: 1H2L
                             RELATED DB: PDB
REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1H2M RELATED DB: PDB
REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1H2N RELATED DB: PDB
```

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REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
          WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900
REMARK 900 RELATED ID: 1L8C
                             RELATED DB: PDB
REMARK 900 STRUCTURAL BASIS FOR HIF-1ALPHA/CBP
          RECOGNITION IN THECELLULAR HYPOXIC RESPONSE
REMARK 900
REMARK 900 RELATED ID: 1LM8
                              RELATED DB: PDB
REMARK 900 STRUCTURE OF A HIF-1A-PVHL-ELONGINB-
REMARK 900 ELONGINC COMPLEX
REMARK 900 RELATED ID: 1LQB
                              RELATED DB: PDB
REMARK 900
           CRYSTAL STRUCTURE OF A HYDROXYLATED HIF-1
REMARK 900 ALPHA PEPTIDEBOUND TO THE PVHL/ELONGIN-C/
REMARK 900 ELONGIN-B COMPLEX
                                 Q969Q7
                                           096907
       1H2K A
               1
                     349 SWS
DBREF
       1H2K S
              786
                     826 SWS
                                 Q16665
                                         HIFA HUMAN
                                                          786
                                                                 826
DBREF
              349
                   MET ALA ALA THR ALA ALA GLU ALA VAL ALA SER GLY SER
SEORES
         1 A
SEORES
         2 A
              349
                   GLY GLU PRO ARG GLU GLU ALA GLY ALA LEU GLY PRO ALA
SEQRES .
              349
                   TRP ASP GLU SER GLN LEU ARG SER TYR SER PHE PRO THR
         3 A
                   ARG PRO ILE PRO ARG LEU SER GLN SER ASP PRO ARG ALA
SEQRES
         4 A
              349
SEORES
         5 A
              349
                   GLU GLU LEU ILE GLU ASN GLU GLU PRO VAL VAL LEU THR
                   ASP THR ASN LEU VAL TYR PRO ALA LEU LYS TRP ASP LEU
SEQRES
         6 A
              349
                   GLU TYR LEU GLN GLU ASN ILE GLY ASN GLY ASP PHE SER
SEQRES
         7 A
              349
                   VAL TYR SER ALA SER THR HIS LYS PHE LEU TYR TYR ASP
SEORES
         8 A
              349
                   GLU LYS LYS MET ALA ASN PHE GLN ASN PHE LYS PRO ARG
SEORES
         9 A
              349
                   SER ASN ARG GLU GLU MET LYS PHE HIS GLU PHE VAL GLU
SEORES
        10 A
              349
SEQRES
        11 A
              349
                   LYS LEU GLN ASP ILE GLN GLN ARG GLY GLY GLU GLU ARG
                   LEU TYR LEU GLN GLN THR LEU ASN ASP THR VAL GLY ARG
SEQRES
        12 A
              349
SEORES
        13 A
              349
                   LYS ILE VAL MET ASP PHE LEU GLY PHE ASN TRP ASN TRP
SEORES
        14 A
              349
                   ILE ASN LYS GLN GLN GLY LYS ARG GLY TRP GLY GLN LEU
SEQRES
        15 A
              349
                   THR SER ASN LEU LEU LEU ILE GLY MET GLU GLY ASN VAL
SEQRES
        16 A
              349
                   THR PRO ALA HIS TYR ASP GLU GLN GLN ASN PHE PHE ALA
                   GLN ILE LYS GLY TYR LYS ARG CYS ILE LEU PHE PRO PRO
SEQRES
        17 A
              349
SEORES
                   ASP GLN PHE GLU CYS LEU TYR PRO TYR PRO VAL HIS HIS
        18 A
              349
SEORES
        19 A
              349
                   PRO CYS ASP ARG GLN SER GLN VAL ASP PHE ASP ASN PRO
SEQRES
        20 A
              349
                   ASP TYR GLU ARG PHE PRO ASN PHE GLN ASN VAL VAL GLY
        21 A
SEORES
              349
                   TYR GLU THR VAL VAL GLY PRO GLY ASP VAL LEU TYR ILE
SEORES
        22 A
              349
                   PRO MET TYR TRP TRP HIS HIS ILE GLU SER LEU LEU ASN
SEORES
        23 A
              349
                   GLY GLY ILE THR ILE THR VAL ASN PHE TRP TYR LYS GLY
        24 A
SEORES
               349
                   ALA PRO THR PRO LYS ARG ILE GLU TYR PRO LEU LYS ALA
SEORES
       25 A
                   HIS GLN LYS VAL ALA ILE MET ARG ASN ILE GLU LYS MET
               349
SEORES
                   LEU GLY GLU ALA LEU GLY ASN PRO GLN GLU VAL GLY PRO
        26 A
               349
SEORES
                    LEU LEU ASN THR MET ILE LYS GLY ARG TYR ASN
       27 A
               349
SEQRES
         1 S
                41
                    SER MET ASP GLU SER GLY LEU PRO GLN LEU THR SER TYR
SEQRES
          2 5
                    ASP CYS GLU VAL ASN ALA PRO ILE GLN GLY SER ARG ASN
                41
SEQRES
          3 S
                    LEU LEU GLN GLY GLU GLU LEU LEU ARG ALA LEU ASP GLN
                41
SEQRES
          4 S
                41
                    VAL ASN
HET
        FE2
            A1350
                        1
HET
        OGA
            A1351
                        10
 HET
        SO4
            A1352
                         5
        SO4
            A1353
 HETNAM
            FE2 FE (II) ION
 HETNAM
            OGA N-OXALYOLGLYCINE
 HETNAM
            SO4 SULFATE ION
 FORMUL
          3
            FE2
                    FE1 2+
 FORMUL
          4
             OGA
                    C4 H5 N1 O5
          5
                    2 (O4 S1 2-)
 FORMUL
             SO4
                   *194 (H2 O1)
 FORMUL
          6
             HOH
              1 ASP A
 HELIX
                        28
                            LEU A
          1
                                    32
              2 ASP A
 HELIX
          2
                        49
                                    58
                            ASN A
                                        1
 HELIX
                        70
                                     76
                                        5
          3
              3 VAL A
                            TRP A
 HELIX
          4
              4 ASP A
                        77
                            ILE A
                                     85
                                        1
          5
              5 ASP A
 HELIX
                       104
                            GLN A
                                   112
```

7

9

```
6 LYS A
HELIX
         6
                       124
                             ARG A
                                    138
                                          1
                                                                                15
             7 GLY A
         7
                       155
                             GLY A
                                     164
HELIX
                                          1
                                                                                10
HELIX
               ASN A
         8
             8
                       166
                             GLY A
                                     178
                                          1
                                                                                 13
HELIX
         9
              9
               PRO A
                       220
                             ASP A
                                     222
                                          5
                                                                                  3
HELIX
        10
             10 GLN A
                       223
                             TYR A
                                     228
                                          1
HELIX
             11 PHE A
                       252
                             VAL A
                                     258
                                          5
                                                                                 7
        11
HELIX
        12
             12 LYS A
                        311
                             GLY A
                                     331
                                          1
                                                                                 21
HELIX
        13
             13 ASN A
                        332
                             GLN A
                                     334
                                          5
                                                                                 3
HELIX
        14
             14 GLU A
                       335
                             LYS A
                                     345
                                          1
                                                                                 11
                             ASP S
HELIX
        15
             15 GLN S
                       814
                                     823
                                          1
                                                                                 10
            AA 5 THR A
SHEET
         1
                        39
                              PRO A
                                     41
                                          n
         2
            AA 5 GLY A 260
SHEET
                              VAL A 265
                                          1
                                             0
                                                 GLY A 260
                                                              N
                                                                 ARG A 40
                                                                 VAL A 265
SHEET
         3
            AA 5 LYS A 214
                              PHE A 219 -1
                                             0
                                                 LYS A 214
                                                              N
SHEET
         4
             AA 5 TRP A 278
                                             0
                                                 TRP A 278
                              SER A 283 -1
                                                              N
                                                                 PHE A 219
                                                                 ILE A 281
SHEET
         5
             AA 5 VAL A 195
                              HIS A 199 -1
                                             0
                                                 THR A 196
                                                              N
             AB 6 ARG A
                         44
SHEET
         1
                              LEU A
                                     45
                                          0
             AB 6 VAL A
SHEET
         2
                          62
                              LEU A
                                                 VAL A
                                                        63
                                                                 LEU A
                                                                         45
                                      64
                                          1
                                             0
                                                              N
             AB 6 VAL A 270
SHEET
         3
                              ILE A 273 -1
                                                 VAL A 270
                                             0
                                                              N
                                                                . LEU A
                                                                        64
SHEET
             AB 6 GLN A 203
                                                 ASN A 205
         4
                              LYS A 211 -1
                                             0
                                                              N
                                                                 ILE A 273
         5
             AB 6 THR A 290
SHEET
                              LYS A 298 -1
                                             0
                                                 ILE A 291
                                                              N
                                                                 ILE A 210
SHEET
         6
             AB 6 LEU A 182
                              SER A 184
                                         -1
                                             N
                                                 THR A 183
                                                              0
                                                                 TRP A 296
SHEET
         1
             AC 9 ARG A
                          44
                              LEU A
                                      45
             AC 9 VAL A
SHEET
         2
                          62
                              LEU A
                                      64
                                                 VAL A
                                                         63
                                                                 LEU A
                                                                         45
                                          1
                                              0
                                                              N
SHEET
          3
             AC 9 VAL A 270
                              ILE A 273
                                                 VAL A 270
                                                                 LEU A
                                         -1
                                              0
                                                              N
                                                                         64
SHEET
             AC 9 GLN A 203
                              LYS A 211 -1
                                                 ASN A 205
                                                                 ILE A 273
          4
                                              0
                                                              N
SHEET
          5
             AC 9 THR A 290
                              LYS A 298 -1
                                                 ILE A 291
                                              0
                                                              N
                                                                  ILE A 210
SHEET
          6
             AC 9 LEU A 186
                              GLY A 190 -1
                                              0
                                                 LEU A 186
                                                              N
                                                                 ASN A 294
SHEET
          7
             AC 9 ARG A 143
                              THR A 149 -1
                                              0
                                                 LEU A 146
                                                              N
                                                                  ILE A 189
             AC 9 PHE A 90
                                                        91
SHEET
          8
                              ALA A 95 -1
                                              0
                                                 SER A
                                                              N
                                                                  GLN A 147
SHEET
             AC 9 SER A 118
                              MET A 123 -1
                                              0
                                                 ASN A 119
                                                                  SER A
                                                                         94
                                                              N
LINK
             FE
                  FE2 A1350
                                               NE2 HIS A 199
                                                                   1555
                                                                                 2.12
                                                                          1555
                  FE2 A1350
LINK
                                               OD2 ASP A 201
                                                                                 2.05
             FE
                                                                   1555
                                                                          1555
                  FE2 A1350
                                               NE2 HIS A 279
                                                                                 2.08
LINK
             FE
                                                                   1555
                                                                           1555
                                                                   1555
LINK
             FΕ
                  FE2 A1350
                                               O2 OGA A1351
                                                                           1555
                                                                                 2.13
                                              · 02' OGA A1351
                  FE2 A1350
LINK
             FE
                                                                   1555
                                                                           1555
                                                                                 2.17
          1 TYR A
                   308
                           PRO A 309
                                                           -1.09
CISPEP
                                                 0
          1 FE1 3 HIS A 199
                               ASP A 201
                                            HIS A 279
SITE
          1 OGA 11 TYR A 145
                                THR A 196
SITE
                                            HIS A 199
                                                        ASP A 201
          2 OGA 11 ASN A 205
                                PHE A 207
SITE
                                            LYS A 214
                                                        HIS A 279
SITE
          3 OGA 11 ILE A 281
                               ASN A 294
                                            TRP A 296
SITE
          1 SO1
                  4 ARG A 138
                                GLY A 140
                                            GLU A 141
                                                        GLU A 142
          1 SO2
                 5 ARG A 143
                                GLU A 192
SITE
                                            GLY A 193
                                                        LEU A 285
                 5 ASN A 286
SITE
          2 SO2
                                              90.00 90.00 P 41 21 2
CRYST1
          86.161
                    86.161 146.656 90.00
ORIGX1
             1.000000
                        0.000000
                                   0.000000
                                                     0.00000
ORIGX2
             0.000000
                        1.000000
                                   0.000000
                                                     0.00000
ORIGX3
             0.000000
                        0.000000
                                   1.000000
                                                     0.00000
             0.011606 0.000000
SCALE1
                                   0.000000
                                                     0.00000
SCALE2
             0.000000
                       0.011606
                                   0.000000
                                                     0.00000
SCALE3
             0.000000
                       0.000000
                                   0.006819
                                                     0.00000
MOTA
           1
              N
                   GLU A 15
                                    8.429 32.653
                                                     9.844
                                                             1.00 50.99
                                                                                     N
ATOM
           2
              CA
                   GLU A
                                    7.077
                                            32.034
                          15
                                                      9.723
                                                             1.00 51.05
                                                                                     C
ATOM
           3
              С
                   GLU A
                          15
                                    7.166
                                           30.582
                                                     10.163
                                                             1.00 50.79
                                                                                     C
ATOM
           4
              0
                   GLU A
                          15
                                    8.052 29.857
                                                      9.730
                                                             1.00 51.18
                                                                                     0
           5
MOTA
              CB
                   GLU A
                          15
                                    6.570
                                           32.124
                                                      8.296
                                                              1.00 51.20
                                                                                     С
MOTA
           6
                   PRO A
                                    6.254
                                            30.150
              N
                          16
                                                     11.022
                                                              1.00 50.50
                                                                                     N
           7
MOTA
              CA
                   PRO A
                          16
                                    6.301
                                            28.781
                                                     11.549
                                                              1.00 50.12
MOTA
           8
              C
                   PRO A
                                    6.265
                                            27.737
                          16
                                                     10.438
                                                              1.00 49.56
                                            27.827
           9
                   PRO A
                                    5.471
MOTA
              0
                          16
                                                      9.503
                                                              1.00 49.32
          10
              CB
                   PRO A
                                    5.049
                                            28.701
ATOM
                          16
                                                     12.429
                                                              1.00 50.27
MOTA
          11
              CG
                   PRO A
                          16
                                    4.734
                                            30.135
                                                     12.770
                                                              1.00 50.58
```

ATOM	12	CD	PRO A	16	5.108	30.911	11.548	1.00 50.56	С
ATOM	13	N	ARG A	17	7.133	26.746	10.550	1.00 48.83	N
ATOM	14	CA	ARG A	17	7.219	25.695	9.550	1.00 48.33	C
ATOM	15	С	ARG A	17	5.967	24.832	9.561	1.00 47.48	С
ATOM	16		ARG A	17	5.245	24.782	10.557	1.00 47.64	0
ATOM	17		ARG A	17	8.421	24.798	9.835	1.00 48.61	С
ATOM	18	CG	ARG A	17	9.776	25.511	9.835	1.00 49.21	С
ATOM	19	CD	ARG A	17	10.944	24.577	10.196	1.00 49.84	C
ATOM	20	NE	ARG A	17	10.918	24.137	11.596	1.00 50.12	Ŋ
ATOM	21	CZ	ARG A	17	11.455	24.809	12.623	1.00 50.99	C
			ARG A	17	12.065	25.979	12.431	1.00 50.40	N
ATOM	22				11.381	24.310	13.857	1.00 50.40	N
ATOM	23		ARG A	17	5.723	24.310	8.446	1.00 46.05	N
ATOM	24	N	GLU A	18					C
ATOM	25		GLU A	18	4.603	23.246	8.329	1.00 45.06	
MOTA	26	С	GLU A	18	5.096		8.607	1.00 44.00	C
MOTA	27	0	GLU A	18	6.101	21.405	8.044	1.00 43.89	0
MOTA	28	CB	GLU A	18	4.013	23.324	6.923	1.00 45.21	C
MOTA	29	CG	GLU A	18	3.323	24.648	6.621	1.00 45.56	C
MOTA	30	CD	GLU A	18	1.951	24.780	7.265	1.00 45.64	С
MOTA	31	OE1	GLU A	18	1.342	23.749	7.641	1.00 44.14	0
MOTA	32	OE2	GLU A	18	1.480	25.932	7.388	1.00 45.83	0
ATOM	33	N	GLU A	19 .	4.396	21.113	9.484	1.00 42.49	N
ATOM	34	CA	GLU A		4.734	19.728	9.795	1.00 41.55	С
ATOM	35	C	GLU A		4.357	18.817	8.635	1.00 39.79	C
ATOM	36	ō	GLU A		3.266	18.933	8.066	1.00 39.13	0
ATOM	37	СВ	GLU A		4.010	19.256	11.052	1.00 41.88	С
ATOM	38	CG	GLU A		4.420	19.997	12.311	1.00 44.80	C
ATOM	39	CD	GLU A		4.276	19.155	13.574	1.00 49.28	Č
ATOM	40	OE1			3.759	18.008	13.497	1.00 51.52	Ō
					4.695	19.643	14.656	1.00 52.76	Ö
ATOM	41		GLU A		5.270	17.910	8.311	1.00 32.70	N
ATOM	42	N	ALA A						C
ATOM	43	CA	ALA A		5.099	16.952	7.227	1.00 36.77	- C
ATOM ·	44	С	ALA A		3.803	16.168	7.373	1.00 35.56	
MOTA	45	0	ALA A		3.445	15.734.		1.00 35.74	0
MOTA	46	CB	ALA A		6.283		7.180	1.00 36.63	C
ATOM	47	N	GLY A		3.082		6.279	1.00 34.05	N
ATOM	48	CA	GLY A		1.860		6.307	1.00 33.24	C
ATOM	49	С	GLY A		0.666		6.551	1.00 32.36	C
MOTA	50	0	GLY P		-0.393		6.951	1.00 30.93	0
MOTA	51	N	ALA A		0.867		6.323	1.00 32.41	N
MOTA	52	CA	ALA A		-0.184		6.459	1.00 32.78	.C
MOTA	53	С	ALA A	22	-0.723		7.873		С
MOTA	54	0	ALA A	22	-1.915	18.605	8.088		0
ATOM	55	CB	ALA A	22	-1.304	18.139	5.462	1.00 32.61	С
ATOM	56	N	LEU A	23	0.151	18.253	8.849	1.00 34.01	N
MOTA	57	CA	LEU A	A 23	-0.297	18.275	10.232	1.00 34.91	С
MOTA	58	C	LEU A	A 23	-0.342	19.694	10.757	1.00 35.27	C
ATOM	59	0	LEU A		-0.528		11.943	1.00 35.72	0
MOTA	60	СВ	LEU A		0.565				С
ATOM	61	CG	LEU A		0.384				С
MOTA	62		LEU Z		1.211				С
ATOM	63		LEU		-1.077				С
MOTA	64	N	GLY 2		-0.177				N
ATOM	65	CA	GLY Z		-0.332				C
					0.901				Č
MOTA	66	C	GLY A						0
ATOM	67	0	GLY I		1.945				N
ATOM	68	N	PRO I		. 0.764				
ATOM	. 69	CA	PRO I		1.896				C
MOTA	70		PRO I		2.327				C
ATOM	71	0	PRO 2		1.488				0
ATOM	72	CB	PRO I	A 25	1.341	26.047	12.043	1.00 36.15	С

MOTA	73	CG	PRO A	A 25	-0.162	25.942	11.982	1.00 35.84	С
ATOM	74	CD	PRO A	A 25	-0.504	24.638	11.350	1.00 36.22	c
ATOM	75	N	ALA A	A 26	3.632	23.848	13.285	1.00 36.64	N
ATOM	76	CA	ALA A	A 26	4.178	23.274	14.499	1.00 37.19	С
ATOM	77	С	ALA A		3.860	24.172	15.706	1.00 36.77	С
ATOM	78	0	ALA A		3.595	23.678	16.808	1.00 37.19	0
MOTA	79	CB	ALA A	A 26	5.672	23.099	14.347	1.00 37.52	С
ATOM	80	N	TRP A		3.848	25.479	15.484	1.00 35.62	N
ATCM	81	CA	TRP A	A 27	3.520	26.420	16.543	1.00 35.04	С
MOTA	82	С	TRP A		3.029	27.729	15.933	1.00 34.20	С
ATOM	83	0	TRP A		2.992	27.883	14.723	1.00 33.57	0
ATOM	84	CB	TRP A		4.774	26.672	17.382	1.00 35.28	С
ATOM	85	CG	TRP A		5.951	26.889	16.511	1.00 34.67	С
ATOM	86	CD1	TRP I		6.761	25.930	15.955	1.00 35.52	С
ATOM	87		TRP		6.426	28.135	16.033	1.00 34.40	С
ATOM	88		TRP 2		7.723	26.522	15.172	1.00 35.09	N
ATOM	89	CE2			7.541	27.877	15.209	1.00 34.23	С
ATOM	90	CE3	TRP 7		6.038	29.452	16.232	1.00 34.31	C
ATOM	91		TRP 2		8.255	28.879	14.592	1.00 35.79	С
ATOM ATOM	92		TRP 2		6.750	30.442	15.629	1.00 36.35	С
ATOM	93 94	CH2			7.847	30.154	14.808	1.00 36.47	C
ATOM	95	N ·	ASP ASP		2.638	28.672	16.766	1.00 33.77	N
ATOM	96	C	ASP :		2.259	29.970	16.249	1.00 33.48	C
ATOM	97	Ö	ASP :			31.050 30.791	17.165 18.276	1.00 32.26	
ATOM	98	CB	ASP .			30.791	16.037	1.00 32.05 1.00 34.30	0
ATOM	99	CG	ASP .			29.986	17.317	1.00 34.30	C
ATOM	100		ASP .			31.027	18.002	1.00 30.29	0
ATOM	101		ASP .			28.906	17.712	1.00 39.78	0
ATOM	102	N	GLU .			32.268	16.654	1.00 33.70	N
ATOM	103	CA	GLU			33.465	17.326	1.00 30.15	c
ATOM	104	С	GLU			33.625	18.752	1.00 28.85	č
ATOM	105	0	GLU			34.036	19.621	1.00 28.58	Ö
ATOM	106	CB	GLU	A 29		34.682	16.503	1.00 30.32	Č
ATOM	107	N	SER	A 30	1.414	.33.313	18.992	1.00 27.95	N
ATOM	108	CA	SER	A 30	0.845	33.501	20.320	1.00 27.46	· C
ATOM	109	С	SER			32.671	21.389	1.00 26.93	С
ATOM	110	0	SER			32.907	22.567	1.00 26.79	0
ATOM	111	CB	SER			33.168	20.322	1.00 27.23	C
ATOM	112	OG	SER			31.764	20.306	1.00 27.69	0
ATOM	113	N	GLN			31.703	20.984	1.00 26.55	N
MOTA	114	CA	GLN			30.837	21.926	1.00 26.63	С
ATOM	115	C	GLN			31.409	22.334	1.00 26.66	С
MOTA	116	0	GLN			30.855	23.205	1.00 26.45	0
MOTA MOTA	117 118	CB	GLN			29.426	21.349	1.00 26.41	С
MOTA	119	CG	·GLN			28.637	21.131	1.00 26.28	С
MOTA	120	CD	GLN GLN			27.287	20.489	1.00 26.25	C
ATOM	121		GLN			27.183	19.271	1.00 27.92	0
ATOM	122	NEZ	LEU			26.258	21.305	1.00 24.36	N
ATOM	123	CA	LEU			32.508 33.176	21.703	1.00 26.89	N
ATOM	124	C	LEU			34.321	22.029 23.006	1.00 27.24	C
ATOM	125	Õ	LEU			35.047	23.006	1.00 26.92 1.00 26.42	C
ATOM	126	СВ	LEU			33.746	20.760	1.00 26.42	. 0
ATOM	127	ÇG	LEU			32.728	19.640	1.00 27.46	C
ATOM	128		LEU			33.391	18.452	1.00 28.65	C
ATOM	129		LEU			31.573	20.127	1.00 29.44	C C
ATOM	130	N	ARG			34.472	23.995	1.00 27.38	Ŋ
ATOM	131	CA	ARG			35.596	24.923	1.00 26.71	N C
ATOM	132	С	ARG			36.880	24.209	1.00 26.57	C
ATOM	133	0	ARG			36.844	23.203	1.00 26.30	ŏ
									•

ATOM	134	CB Z	ARG A	. :	33	•	7.492	35.357	26.163	1.00			С
ATOM	135	CG 2	ARG A	. :	33	•	7.052	34.141	26.983	1.00			С
ATOM	136	CD 2	ARG A	. :	33		7.937	33.837	28.181	1.00			С
ATOM	137	NE :	ARG A	. :	33		7.381	32.778	29.018	1.00			N
ATOM	138	CZ :	ARG A		33		6.451	32.946	29.945	1.00			С
ATOM	139	NH1	ARG A	1	33		5.937	34.140	30.189	1.00			N
ATOM	140		ARG A		33		6.029	31.901	30.637	1.00	25.35		N
ATOM	141		SER F		34		6.633	38.020	24.732	1.00	26.80		N
ATOM	142		SER F		34		6.903	39.280	24.061		27.15		С
ATOM	143		SER F		34		7.990	40.048	24.791	1.00	26.39		С
ATOM	144		SER A		34		7.964	40.140	26.005	1.00	25.87		0
ATOM	145		SER A		34		5.628	40.104	24.030		27.68		С
ATOM	146		SER A		34		5.494	40.737	25.285	1.00	32.47		0
MOTA	147		TYR A		35		8.944	40.589	24.042		25.89		И.
MOTA	148		TYR A		35	1	0.110	41.223	24.637		26.28		С
ATOM	149	С	TYR A	A.	35	1	.0.353	42.558	23.970		26.85		С
MOTA	150	0	TYR A	A	35		9.722	42.856	22.967		26.92		0
ATOM	151	CB	TYR Z	A	35	1	1.326	40.308	24.510		25.90		C
MOTA	152	CG	TYR I	A	35	1	11.169	39.032	25.309		25.33		C
ATOM	153		TYR 2	A	35	1	LO.975	39.073	26.685		24.99		C
ATOM	154		TYR .		35	3	L1.198	37.787	24.692		23.82		С
MOTA	155	CE1	TYR .	Α	35	1	10.823	37.898	27.429		24.56		С
ATOM	156	CE2	TYR .	Α	35	-	11.046	36.620	25.426		24.42		С
ATOM	157	CZ	TYR .	A	35	:	10.862	36.682	26.793		23.48	-	С
ATOM	158	OH	TYR	Α	35	:	10.696	35.524	27.513		24.75		0
ATOM	159	N	SER	Α	36	:	11.304	43.327	24.496		27.27		N
ATOM	160	CA	SER	Α	36		11.525	44.704	24.052		27.55		С
ATOM	161	С	SER	Α	36		12.513	44.912	22.917		27.06		С
MOTA	162	0	SER	Α	36		12.734	46.049	22.504		27.94		0
MOTA	163	CB	SER	Α	36		12.082	45.498	25.226		27.88		C
MOTA	164	OG	SER	Α	36		13.350	44.976	25.590		28.36		0
ATOM	165	N	PHE	Α	37		13.128	43.851	22.429		25.35		N
ATOM	166	CA	PHE	Α	37		14.202		21.461		24.62		C
MOTA	167	C	PHE	Α	37		13.899		20.159		24.75		С
MOTA	168	0	PHE	Α	37		13.130				24.25		0
MOTA	169	CB	PHE	Α	37		15.487				23.87		C
MOTA	170	CG	PHE		37		15.318				22.53		С
MOTA	171		PHE		37		15.348				21.11		C
MOTA		. CD2					15.069				21.63		C C
ATOM .	173		PHE		37		15.158				22.41		C
MOTA	174	CE2	PHE		37		14.900				22.29		C
MOTA	175		PHE		37		14.936				21.45		
MOTA	176		PRO		38		14.489				24.94		N C
MOTA	177		PRO		38		14.322		_		24.67		C
MOTA	178		PRO		38		15.267				24.41		o
MOTA	179		PRO		38		16.249				23.75		c
MOTA	180		PRO		38		14.725				26.09		c
ATOM	181		PRO		38		15.791				25.27		c
MOTA	182		PRO		38		15.287				23.27		N
MOTA	183		THR		39		14.981				0 23.42		C
ATOM	184		THR		39		15.859				0 24.29		Ċ
ATOM	185		THR		39		15.857				0 24.29		Ö
MOTA	186		THR		39		14.958				0 24.01		C
MOTA	187		THR		39		15.368				0 19.92		o
ATOM	188		1 THR				14.044				0 23.03		Č
ATOM	189		2 THR				15.213				0 23.03		N
ATOM	190		ARG				16.854				0 24.43		Ċ
MOTA	191						16.982 17.063				0 24.49		. c
MOTA	192		ARG				17.434				0 23.58		ō
ATOM	193 194		ARG ARG				18.25				0 25.36		Ċ
MOTA	19,	. CB	UAR	, A	40		10.23.	5 55.00.			3.50		_

ATOM	195	CG	ARG	A	40	18.208	40.281	12.248	1.00 30.	74
ATOM	196	CD	ARG	Α	40	16.823	40.775	11.890	1.00 30.	
ATOM	197	NE	ARG		40	16.604	40.989	10.477		
ATOM	198	CZ	ARG		40	15.403			1.00 39.	
ATOM	199	NH1			40	14.345	41.229	9.971	1.00 43.	
ATOM	200		ARG				41.254	10.782	1.00 45.	
ATOM	201				40	15.252	41.457	8.674	1.00 44.	
		N	PRO		41	16.687	36.031	12.221	1.00 25.	
MOTA	202	CA	PRO		41	16.715	34.565	12.290	1.00 25.	
ATOM	203	C	PRO		41	18.095	33.913	12.282	1.00 25.	.10
ATOM	204	0	PRO		41	19.007	34.370	11.636	1.00 25.	.16
ATOM	205	CB	PRO		41	15.953	34.130	11.023	1.00 25.	.76
ATOM	206	CG	PRO	Α	41	15.286	35.392	10.504	1.00 26.	
ATOM	207	CD	PRO	A	41	16.151	36.524	10.939	1.00 24.	
ATOM	208	N	ILE	A	42	18.225	32.823	13.020	1.00 25.	
MOTA	209	CA	ILE	Α	42	19.388	31.974	12.919	1.00 24.	
ATOM	210	C	ILE	A	42	19.147	31.116	11.677	1.00.24.	
ATOM	211	0	ILE		42	18.043	30.614	11.466	1.00 24.	
ATOM	212	CB	ILE		42	19.481	31.104	14.163	1.00 24.	
ATOM	213		ILE		42	19.763	31.993	15.384		
ATOM	214		ILE		42	20.530	30.004	13.364	1.00 24.	
ATOM	215		ILE		42	19.531	31.325		1.00 23.	
ATOM	216	N	PRO		43			16.729	1.00 23.	
ATOM	217	CA	PRO		43	20.146	30.953	10.826	1.00 24.	
ATOM	218	C	PRO			19.963	30.108	9.651	1.00 24.	
ATOM	219	o			43	19.611	28.650	10.001	1.00 24.	
ATOM	220		PRO		43	20.148	28.130	10.989	1.00 24.	
		CB	PRO		43	21.320	30.192	8.937	1.00 24.	
ATOM	221	CG	PRO		43	22.040	31.372	9.541	1.00 25.	
ATOM	222	CD	PRO		43	21.475	31.583	10.886	1.00 24.	. 37
ATOM	223	N	ARG		44	18.686	28.032	9.248	1.00 24.	.70
ATOM	224	CA	ARG		44	18.367	26.608	9.391	1.00 25.	. 53
MOTA	225	С	ARG	A	44	18.910	25.943	8.152	1.00 25.	.00
ATOM	226	0	ARG	Α	44	18.505	26.265	7.030	1.00 24.	
ATOM	227	CB	ARG	Α	44	16.873	26.287	9.452	1.00 26.	
MOTA	228	CG	ARG	A	44	16.044	27.133	10.378	1.00 29.	
MOTA	229	CD	ARG	A	44	·14.683	26.485	10.813	1.00 31.	
MOTA	230	NE	ARG	A	44	14.401	25.120	10.323	1.00 32.	
MOTA	231	CZ	ARG	A	44	14.174	24.057	11.126	1.00 33.	
ATOM	232	NH1	ARG		44 .	14.239	24.170	12.451	1.00 30.	
ATOM	233		ARG		44	13.898	22.863	10.613	1.00 30.	
ATOM	234	N	LEU		45	19.815	25.006	8.337		
ATOM	235	CA	LEU		45	20.500	24.444		1.00 23.	
ATOM	236	C	LEU		45	20.684		7.202	1.00 23.	
ATOM	237	ō	LEU		45		22.967	7.352	1.00 23.	
ATOM	238	СВ	LEU		45	20.559 21.888	22.423	8.446	1.00 22.	
ATOM	239	CG	LEU				25.064	7.093	1.00 22.	
ATOM	240		LEU		45	21.911	26.563	6.819	1.00 23.	
ATOM	241				45	23.317	27.111	6.947	1.00 24.	
			LEU		45	21.366	26.845	5.423	1.00 24.	
MOTA	242	N	SER		46	21.018	22.347	6.227	1.00 23.	
ATOM	243	CA	SER		46	21.382	20.975	6.221	1.00 24.	.12
ATOM	244	С	SER		46	22.820	20.888	6.668	1.00 24.	.81
ATOM	245	0	SER	Α	46	23.640	21.757	6.398	1.00 23.	
ATOM	246	CB	SER		46	21.236	20.354	4.830	1.00 23.	
ATOM	247	OG	SER	Α	46	21.744	19.020	4.830	1.00 24.	
ATOM	248	N	GLN	A	47	23.089	19.804	7.366	1.00 25.	
MOTA	249	CA	GLN		47	24.399	19.444	7.844	1.00 27.	
ATOM	250	С	GLN		47	25.379	19.326	6.674	1.00 27.	
ATOM	251	0	GLN		47	26.563	19.564	6.836	1.00 27.	
ATOM	252	CB	GLN		47	24.245	18.088	8.554		
ATOM	253	CG	GLN		47	25.487	17.279		1.00 28.	
ATOM	254	CD	GLN		47	25.776		8.705	1.00 31.	
ATOM	255		GLN		47	24.881	16.372	7.570	1.00 33.	
				**	• •	74.00I	15.970	6.803	1.00 36.	23

							_		2 450	1 00 3	C 17		N
MOT			SLN A		17	27.041	_	6.000	7.458	1.00 3			N
MOTA	257	•	SER A		18	24.884		8.951	5.498	1.00 2			C
ATOM	258		SER A		18	25.736		8.809	4.323	1.00 2			Ċ.
ATOM	259		SER A		48	26.016		0.150	3.629	1.00 2			Ö
ATOM	260		SER A		48	26.825		20.235	2.711	1.00 2			C
MOTA	261		SER A		48	25.092		.7.839	3.324	1.00 2			0
ATOM	262		SER A		48	23.798		L8.276	2.918	1.00 2			N
ATOM	263	N .	ASP A	7	49	25.347		21.203	4.065	1.00			
ATOM	264	CA	ASP A	7	49	25.515		22.496	3.442	1.00		•	C
MOTA	265	C .	ASP F	Į.	49	26.800		23,163	3.913	1.00			C
MOTA	266	0	ASP A	7	49	26.981		23.398	5.101	1.00			0 C
ATOM	267	CB	ASP A	4	49	24.325		23.369	3.783	1.00			
ATOM	268	CG	ASP A	Ą	49	24.316		24.667	3.010	1.00			C
ATOM	269	OD1	ASP A	4	49	25.398		25.183	2.666	1.00			0
ATOM	270	OD2	ASP A	A	49	23.259		25.247	2.731	1.00			0
ATOM	271	N	PRO A	A	50	27.693		23.483	2.976	1.00			И
ATOM	272	CA	PRO 2	Α.	50	28.964		24.134	3.315	1.00			C
ATOM	273	С	PRO I	A	50	28.783		25.354	4.186		30.38		C
MOTA	274	0	PRO I	A	50	29.663		25.651	4.990		30.53		0
ATOM	275	CB.	PRO I	Α	50	29.520		24.573	1.952		30.39		C
MOTA	276	CG	PRO .	A	50	28.926		23.667	0.988		30.96		C
MOTA	277	CD	PRO :	A	50	27.57	1	23.243	1.531		30.51		C
MOTA	278	N	ARG	A	51	27.683	3	26.072	4.008		30.50		N
ATOM	279	CA	ARG	Α	51	27.43	9	27.253	4.817		30.94		C
ATOM	280	С	ARG	Α	51	27.34		26.875	6.299		30.49		C
ATOM	281	0	ARG	Α	51	27.74	4	27.646	7.161		29.74		0
MOTA	282	CB	ARG	A	51	26.17	1.	27.979	4.370		30.97		C
MOTA	283	CG	ARG	A	51	26.33	7	28.781	3.099		33.47		C
MOTA	284	CD	ARG	Α	51	25.02	9	29.321	2.521		34.80		C
ATOM	285	NE	ARG	Α	51	24.07	1	28.252	2.221		36.68		N
MOTA	286	CZ	ARG		51	22.76	6	28.448	2.081		37.94		C
MOTA	287		ARG		51	22.26	0	29.677	2.208		39.10		N
ATOM	288		ARG		51	21.96	7	27.436	1.794		36.51		N
MOTA	289	N	ALA	Α	52	26.83		25.684	6.596		30.03		N
ATOM	290	CA	ALA		52	26.69	7	25.288	7.993		29.96		C
MOTA	291		ALA	A	52	28.07	9	25.101	8.593		30.07		C
ATOM	292		ALA	Α	52	28.34	5	25.518	9.710		29.00		0
MOTA	293		ALA	A	52	25.90	1	24.028	8.119		29.81		C
MOTA	294		GLU	A	53	28.95	8	24.455	7.845		30.12		N
MOTA	295		GLU	A	53	30.29	90	24.213	8.347		31.08		C
ATOM	296		GLU	A	53	30.99		25.550	8.579		30.37		C
ATOM	297		GLU	Α	53	31.68		25.730	9.580		29.89		0
ATOM	298		GLU	A	53	31.08		23.362	7.379		31.41		C
MOTA	299		GLU	Α	53	32.18		22.603	8.081		35.02		. С
MOTA	300		GLU	A	53	31.78	35	21.185	8.507		37.87		C
ATOM	301	OE	1 GLU	Α	53	30.6		20.929	8.887		39.16		0
ATOM	302	OE	2 GLU	Α	53	32.6		20.313	8.463		40.43		0
MOTA	303		GLU		54	30.8		26.479	7.652		29.84		N
MOTA	304				54	31.4	13	27.796	7.757		30.22		C
MOTA	305		GLU	A	54	30.9	75	28.486	9.049		29.05		C
MOTA	306		GLU	A	54	31.7		29.102	9.71		28.03		C
MOTA	307				54	31.0		28.680	6.57		30.53		
· ATOM	308				54	31.6		28.276			34.66		
MOTA	30				54	30.9	93	29.002			38.49		
MOTA	. 310		1 GLU			30.6		30.208			0 42.20		
ATOM	31:		2 GLU			30.8		28.368			0 41.54		-
MOTA	31:		LEU			29.6		28.366			0 28.24		ľ
ATOM	31					29.1	77	29.029			0 27.28		(
MOTA	31		LEC			29.7	74	28.448			0 26.43		(
ATOM	31		LEU			30.2					0 25.20		(
MOTA	31					27.6	55	28.975	10.59	7 1.0	0 27.25		(

ATOM	317	CG	LEU A	55	27.027	29.829	9.502	1.00 27.43
ATOM	318	CD1	LEU A	55	25.568	29.452	9.322	1.00 28.83
ATOM	319	CD2	LEU A	55	27.173	31.318	9.821	1.00 26.98
ATOM	320	N	ILE A	56	29.829	27.116	11.915	1.00 25.75
ATOM	321	CA	ILE A	56	30.382	26.473	13.107	
ATOM	322	C	ILE A	56	31.874	26.815		1.00 25.50
ATOM	323	ō	ILE A	56	32.346		13.254	1.00 26.26
ATOM	324	СВ	ILE A	56	32.340	27.134	14.349	1.00 25.55
ATOM	325	CG1			30.192	24.955	13.059	1.00 25.63
ATOM	326				28.698	24.574	13.034	1.00 24.00
ATOM		CG2		56	30.848	24.321	14.263	1.00 25.48
	327	CD1		56	28.439	23.170	12.531	1.00 24.10
ATOM	328	N	GLU A	57	32.597	26.781	12.135	1.00 27.04
ATOM	329	CA	GLU A	57	34.023	27.082	12.107	1.00 28.01
ATOM	330	С	GLU A	57	34.232	28.491	12.625	1.00 28.49
MOTA	331	0	GLU A	57	35.183	28.770	13.344	1.00 28.92
MOTA	332	CB	GLU A	57	34.561	26.977	10.676	1.00 28.61
MOTA	333	CG	GLU A	57	36.053	27.224	10.509	1.00 30.77
ATOM	334	CD	GLU A	57	36.902	26.322	11.394	1.00 35.15
MOTA	335	OE1		57	36.556	25.127	11.591	
ATOM	336	OE2		57	37.924	26.818		1.00 37.11
ATOM	337	N	ASN A	58	33.321	29.378	11.909	1.00 40.88
ATOM	338	CA	ASN A	58	33.424		12.270	1.00 28.34
ATOM	339	C	ASN A	58		30.758	12.701	1.00 28.81
ATOM	340	Õ	ASN A		32.770	31.079	14.025	1.00 27.23
ATOM	341	СВ		58	. 32.630	32.233	14.374	1.00 26.07
ATOM			ASN A	58	32.792	31.641	11.656	1.00 29.66
	342	CG	ASN A	58	33.789	32.386	10.913	1.00 33.61
ATOM	343	OD1		58	34.280	31.901	9.893	1.00 38.81
ATOM	344	ND2		58	34.160	33.582	11.429	1.00 36.72
ATOM	345	N	GLU A	59	32.343	30.053	14.735	1.00 26.39
ATOM	346	CA	GLU A	59	31.712	30.241	16.030	1.00 26.36
ATOM	347	С	GLU A	59	30.495	31.144	15.926	1.00 25.39
ATOM	348	0	GLU A	59	30.325	32.100	16.668	1.00 24.14
ATOM	349	CB	GLU A	59	32.753	30.697	17.059	1.00 26.80
MOTA	350	CG	GLU A	59	33.717	29.537	17.316	1.00 29.10
ATOM	351	CD	GLU A	59	34.722	29.791	18.407	1.00 29.10
MOTA	352	OEl		59	35.790	30.330	18.080	
ATOM	353	OE2		59	34.466	29.432	19.572	1.00 37.47
ATOM	354	N	GLU A	60	29.641			1.00 34.14
ATOM	355	CA	GLU A	60	28.366	30.799	14.970	1.00 24.88
ATOM	356	C	GLU A	60	27.262	31.465	14.801	1.00 25.20
ATOM	357	Ö	GLU A	60		30.414	14.822	1.00 24.07
ATOM	358	СВ	GLU A		27.420	29.320	14.293	1.00 22.49
ATOM	359	CG		60	28.343	32.249	13.505	1.00 25.69
ATOM	360		GLU A	60	29.354	33.363	13.536	1.00 30.40
ATOM	361	CD	GLU A	60	28.962	34.516	12.657	1.00 37.91
		OE1		60	29.009	34.377	11.414	1.00 38.24
ATOM	362		GLU A	60	28.595	35.566	13.236	1.00 46.50
ATOM	363	N	PRO A	61	26.124	30.779	15.386	1.00 22.90
ATOM	364	CA	PRO A	61 -	25.045	29.816	15.571	1.00 22.19
ATOM	365	С	PRO A	61	24.448	29.371	14.267	1.00 21.47
ATOM	366	0	PRO A	61	24.419	30.104	13.266	1.00 20.48
ATOM	367	CB	PRO A	61	23.996	30.583	16.368	1.00 22.29
ATOM	368	CG	PRO A	61	24.315	32.053	16.148	
ATOM	369	CD	PRO A	61	25.764	32.140	15.798	1.00 22.67
ATOM	370	N	VAL A	62	23.957	28.142		1.00 22.92
ATOM	371	CA	VAL A	62	23.248		14.283	1.00 20.87
ATOM	372	C	VAL A	62	22.353	27.591	13.146	1.00 20.94
ATOM	373	Ö	VAL A	62		26.475	13.655	1.00 21.15
ATOM	374	СВ	VAL A		22.714	25.761	14.605	1.00 21.21
ATOM	375		VAL A	62	24.214	27.052	12.073	1.00 21.30
ATOM	376			62	25.061	25.912	12.608	1.00 22.10
ATOM			VAL A	62	23.440	26.587	10.825	1.00 21.19
VI OM	377	N	VAL A	63	21.158	26.366	13.084	1.00 21.48

		20.302 25.231 13.374 1.00 21.87
MOTA	378 CA VAL A 63	
MOTA	379 C VAL A 63	20.526 24.212 12.270 1.00 22.00
ATOM	380 O VAL A 63	20.366 24.528 11.109 1.00 22.54
ATOM	381 CB VAL A 63	18.793 25.574 13.421 1.00 22.02
	382 CG1 VAL A 63	17.955 24.277 13.612 1.00 21.90
MOTA		18.494 26.522 14.546 1.00 21.22
MOTA	· · ·	
MOTA	384 N LEUA 64	
MOTA	385 CA LEU A 64	
MOTA	386 C LEUA 64	19.826 21.014 11.775 1.00 22.19
MOTA	387 O LEUA 64	19.423 20.558 12.843 1.00 21.85
MOTA	388 CB LEU A 64	22.327 21.107 12.032 1.00 24.00
ATOM	389 CG LEU A 64	23.614 21.930 11.984 1.00 27.02
	390 CD1 LEU A 64	24.791 21.080 12.303 1.00 31.61
ATOM		23.827 22.540 10.640 1.00 29.86
MOTA		19.222 20.757 10.628 1.00 21.50
ATOM	392 N THR A 65	25.00
ATOM	393 CA THR A 65	
MOTA	394 C THR A 65	20,100
MOTA	395 O THR A 65	
MOTA	396 CB THR A 65	17.062 20.592 9.478 1.00 22.08
ATOM	397 OG1 THR A 65	17.725 20.351 8.230 1.00 22.38
ATOM	398 CG2 THR A 65	16.919 22.099 9.553 1.00 24.00
	399 N ASP A 66	19.168 18.062 9.961 1.00 21.50
MOTA		19.259 16.650 9.604 1.00 21.86
MOTA	400 CA ASP A 66 401 C ASP A 66	20.513 15.899 10.069 1.00 21.61
MOTA	-	21.070 15.088 9.316 1.00 21.82
MOTA	402 O ASP A 66	1 22 22 22
MOTA	403 CB ASP A 66	20.000
MOTA	404 CG ASP A 66	
MOTA	405 OD1 ASP A 66	21.065 17.936 8.070 1.00 21.14
MOTA	406 OD2 ASP A 66	20.240 17.477 6.159 1.00 25.40
MOTA	407 N THR A 67	20.967 16.158 11.287 1.00 21.05
ATOM	408 CA THR A 67	22.154 15.491 11.768 1.00 20.85
MOTA	409 C THR A 67	21.858 14.084 12.231 1.00 20.12
MOTA	410 O THR A 67	22.757 13.281 12.283 1.00 20.45
ATOM	411 CB THR A 67	22.747 16.207 12.977 1.00 20.77
	412 OG1 THR A 67	21.782 16.210 14.039 1.00 20.61
MOTA	413 CG2 THR A 67	23.054 17.671 12.682 1.00 22.44
ATOM		20.614 13.815 12.618 1.00 19.51
MOTA		20.269 12.555 13.267 1.00 19.09
MOTA		21.116 12.349 14.517 1.00 18.40
MOTA	416 C ASN A 68	21.383 11.212 14.928 1.00 17.67
MOTA	417 O ASN A 68	
ATOM	418 CB ASN A 68	
MOTA	419 CG ASN A 68	13.100
MOTA	420 OD1 ASN A 68	1 00 10 00
MOTA	421 ND2 ASN A 68	##:# ==: -==
MOTA	422 N LEUA 69	21.532 13.448 15.134 1.00 18.28
ATOM	423 CA LEU A 69	22.378 13.382 16.326 1.00 17.98
MOTA	424 C LEU A 69	21.773 12.542 17.447 1.00 17.59
ATOM	425 O LEU A 69	22.478 11.725 18.039 1.00 17.61
ATOM	426 CB LEU A 69	22.693 14.772 16.844 1.00 18.38
MOTA	427 CG LEU A 69	23.636 14.859 18.035 1.00 18.31
ATOM	428 CD1 LEU A 69	24.936 14.144 17.744 1.00 20.68
		23.907 16.299 18.399 1.00 19.25
MOTA		20.489 12.741 17.740 1.00 17.27
ATOM		19.811 11.989 18.794 1.00 17.72
ATOM		18.588 11.253 18.257 1.00 18.11
MOTA		
ATOM		
ATOM		
ATOM		
MOTA		18.451 13.994 19.599 1.00 17.50
ATOM		18.715 10.764 17.028 1.00 19.22
ATOM		17.615 10.071 16.367 1.00 19.79

.TC.	439	С	TYR		71	16.934	9.072	17.306	1.00 1		(С
MOT.	440	0	TYR		71	15.726	9.120	17.457	1.00 1		(0
MOT.	441	CB	TYR		71	18.082	9.406	15.055	1.00 2			С
MOT.	442	CG	TYR		71	17.156	8.320	14.554	1.00 2			С
T.	443		TYR		71	15.938		13.948	1.00 2			С
MOT.	444		TYR		71	17.503	6.986	14.691	1.00 2			С
MOT.	445 446		TYR TYR		71 71	15.080	7.555	13.480	1.00 2			С
TOM.	447	CZ	TYR		71	16.684 15.479	5.968 6.244	14.252 13.650	1.00 2			C
MOT.	448	OH	TYR		71	14.686	5.159	13.266	1.00 2			С 0
TOM.	449	N	PRO		72	17.688	8.200	17.960	1.00 2			N
MOT.	450	CA	PRO		72	17.074	7.196	18.840	1.00 2			C
MOT.	451	С	PRO		72	16.307	7.794	20.008	1.00 2			č
MOT.	452	0	PRO	A	72	15.463	7.120	20.535	1.00 2			Ō
MOT.	453	CB	PRO	A	72	18.267	6.377	19.351	1.00 2			С
MOT.	454	CG	PRO	A	72	19.362	6.650	18.386	1.00 2	21.75		С
MOT.	455	CD	PRO		72	19.151	8.065	17.905	1.00 2	20.71		С
MOT.	456	N	ALA		73	16.588	9.038	20.391	1.00 2			N
MOT.	457	CA	ALA		73	15.892	9.658	21.522	1.00 2			С
MOT.	458 450	C	ALA		73	14.567	10.293	21.103	1.00 2			С
MOT. MOT.	459 460	O CB	ALA ALA		73	13.801	10.765	21.938	1.00 2			0
MOT.	461	N	LEU		73 74	16.783 14.297	10.718	22.173 19.808	1.00 2			C
TOM.	462	CA	LEU		74	13.086	10.322	19.329	1.00 2			N C
MOT.	463	C	LEU		74	11.797	10.301	19.801	1.00 2			c
MOT.	464	0	LEU		74	10.732		19.746	1.00			Ö
MOT.	465	CB	LEU	A	74	13.114	11.076	17.810	1.00 2			C
MOT.	466	CG	LEU	Α	74	14.185	12.061	17.296	1.00 2	24.67		С
MOT.	467		LEU		74	13.988	12.320	15.820	1.00 2	26.73		С
MOT.	468		LEU		74	14.225	13.371	18.077	1.00	23.39		С
MOT.	469	N	LYS		75	11.897	9.053	20.244	1.00			N
MOT.	470	CA	LYS		75	10.741	8.317	20.738	1.00			С
MOT.	471	С	LYS		75	10.589	8.519	22.245	1.00			Ç
TOM.	472 473	O CB	LYS LYS		75 75	9.612 10.885	8.082	22.822	1.00			0
.TOM	474	CG	LYS		75 75	12.079	6.819 6.163	20.428 21.097	1.00			C C
MOT.	475	CD	LYS		75	12.178	4.653	20.765	1.00		•	c
MOT.	476	CE	LYS		75	13.646	4.220	20.609	1.00		•	c
MOT.	477	NZ	LYS		75	14.348	4.123	21.868	1.00			N
MOT.	478	N	TRP	A	76	11.552	9.179	22.882	1.00			N
MOT.	479	CA	TRP	Α	76	11.486	9.389	24.319	1.00	25.56		С
MOT.	480		TRP		76	10.268	10.201		1.00			С
MOT	481	0	TRP		76	9.920	11.198	24.130	1.00			0
TOM	482	CB ·			76	12.719	10.139	24.816	1.00			C
TOM TOM	483 484	CG	TRP		76	13.975	9.338	24.816	1.00			С
TOM	484		TRP TRP		76 76	14.129	8.059	24.393	1.00			C
TOM	486		TRP		76	15.258 15.431	9.762 7.658	25.271 24.552	1.00			C
TOM	487		TRP		76	16.145	8.685	25.096	1.00			N C
TOM	488		TRP		76	15.750	10.944	25.817	1.00			C
TOM	489		TRP		76	17.481	8.756	25.437	1.00			C
MOT	490	CZ3	TRP	A	76	17.088	11.012	26.163	1.00			c
TOM	491	CH2	TRP		76	17.932	9.934	25.970	1.00			C
TOM	492	N	ASP		77	9.643	9.772	25.836	1.00			N
TOM	493	CA	ASP		77	8.583	10.530	26.467	1.00			С
TOM	494	C	ASP		77	8.618	10.116	27.931	1.00			С
TOM TOM	495	O	ASP		77	9.405	9.264	28.291	1.00			0
TOM	496 497	CB CG	ASP ASP		77 77	7.230	10.276	25.810	1.00			C
TOM	497		ASP		77 77	6.795 7.388	8.835 8.015	25.885 26.638	1.00			C
TOM	499		ASP		77	5.832	8.439	25.211	1.00			0
					• •	3.032	0.409	20.211	1.00	23.31		9

MOTA	500		LEU A		78	7.790	10.705	28.775	1.00 25.96	N
ATOM	501		LEU A		78	7.893	10.441	30.201	1.00 26.27	C
MOTA	502		LEU I		78	7.716	8.965	30.539	1.00 26.14	C 0
ATOM	503		LEU A		78	8.446	8.438	31.374	1.00 25.51	c
ATOM	504		LEU 2		78	6.905	11.301	30.979	1.00 26.32	c
MOTA	505		LEU .		78	7.155	12.802	30.860	1.00 27.35	
ATOM	506		LEU .		78	6.098	13.579	31.623	1.00 28.05	C
MOTA	507		LEU .		78	8.536	13.165	31.379	1.00 28.39	C
MOTA	508	N	GLU		79	6.775	8.297	29.874	1.00 26.56	N C
MOTA	509	CA	GLU		79	6.526	6.876	30.123	1.00 27.00	C
MOTA	510	С	GLU		79	7.754	6.029	29.780	1.00 26.63	o
MOTA	511	0	GLU		79	8.220	5.231	30.583	1.00 25.94 1.00 27.39	c
ATOM	512	CB	GLU		79	5.302	6.371	29.333	1.00 27.39	c
MOTA	513	CG	GLU		79	4.963	4.919	29.657	1.00 29.75	c
MOTA	514	CD	GLU		79	3.803	4.347	28.854 27.863	1.00 35.13	ő
MOTA	515		GLU		79	3.361	4.976	29.224	1.00 35.44	Ö
ATOM	516		GLÜ		79	3.338	3.245 6.205	28.575	1.00 35.44	N
ATOM	517	N	TYR		80	8.279	5.465	28.169	1.00 26.29	c
ATOM	518	CA	TYR		80 .	9.466	5.763	29.072	1.00 25.83	Ċ
ATOM	519	C	TYR		80	10.669	4.863	29.435	1.00 25.75	Ö
MOTA	520	0	TYR		80 .	11.418 9.812	5.802	26.728	1.00 26.53	Ċ
ATOM	521	CB	TYR		80	11.047	5.106	26.210	1.00 26.94	Ċ
MOTA	522	CG	TYR		80	10.971	3.836	25.637	1.00 26.53	Ċ
MOTA	523	CD1			80 80	12.287	5.721	26.291	1.00 25.32	. C
ATOM	524		TYR		80	12.207	3.208	25.142	1.00 26.28	C
MOTA	525 526	CE2	TYR TYR		80	13.416	5.109	25.823	1.00 25.73	Ċ
ATOM ATOM	527	CEZ	TYR		80 .	13.331	3.861	25.240	1.00 25.94	С
ATOM	528	OH	TYR		80	14.478	3.294	24.758	1.00 25.55	0
ATOM	529	N	LEU		81	10.859	7.016	29.448	1.00 25.62	N
ATOM	530	CA	LEU		81	12.000	7.350	30.309	1.00 25.87	С
ATOM	531	C	LEU		81	11.821	6.794	31.733	1.00 26.06	С
ATOM	532	ŏ	LEU		81	12.763	6.263	32.327	1.00 26.00	0
ATOM	533	СВ	LEU		81	12.250	8.863	30.340	1.00 25.81	С
ATOM	534	CG	LEU		81	12.748	9.501	29.030	1.00 25.65	С
ATOM	535		LEU		81	12.828	11.010	29.174	1.00 26.40	C
ATOM	536		LEU		81	14.102	8.959	28.592	1.00 25.79	C
ATOM	537	N	GLN		82	10.617	6.913	32.274	1.00 26.27	N
ATOM	538	CA	GLN	Α	82	10.338	6.388	33.602	1.00 26.77	C
ATOM	539	С	GLN	Α	82	10.640		33.623	1.00 26.51	C
ATOM	540	0	GLN	Α	82	11.232		34.552	1.00 26.60	0
MOTA	541	CB	GLN	A	82	8.877		33.974	1.00 26.90	C
ATOM-	542	CG	GLN	ΙΑ	82	8.466				C
MOTA	543		GLN		82	7.315				C
MOTA	544		1 GLN		82	6.755				0
ATOM	545		2 GLN		82	6.944				N
MOTA	546			JA	83	10.252				N C
ATOM	547			JA	83	10.429				c
MOTA	548			JA	83	11.893				0
MOTA	549			JA		12.285				C
ATOM	550			JA		9.604				c
MOTA	551			JA		9.607				č
MOTA	552			JA		8.902				o
ATOM	553			JA		8.258				Ö
ATOM	554			J A		9.008				N
ATOM	555			N A		12.711 14.063				C
ATOM	556			N A		15.27				C
MOTA	557			N A N A		16.392				ō
ATOM	558 559			n A N A		14.13				c
MOTA	560			N A		13.26				C
MOTA	200	,		., .,						

ATOM	561	OD1	ASN .	A	84	13.402	0.608	29.439	1.00 2	4.26	0	
MOTA	562	ND2	ASN .	A	84	12.354	2.231	28.288	1.00 2	22.66	N	
MOTA	563		ILE .		85	15.087	4.773	32.422	1.00 2		N	
ATOM	564		ILE .		85	16.240	5.599	32.763	1.00 2		C	
ATOM	565		ILE .		85	16.930	5.307	34.099	1.00 2		C	
ATOM	566 563		ILE .		85	17.820	6.054	34.519	1.00 2		0	
ATOM ATOM	567 568		ILE ILE		85 85	15.846 17.049	7.076 7.923	32.688 32.270	1.00 2		C C	
ATOM	569		ILE		85	15.232	7.535	33.988	1.00 2		C	
ATOM	570		ILE		85	16.696	9.389	32.000	1.00		C	
ATOM	571	N	GLY		86	16.503	4.253	34.773	1.00		N	
ATOM	572	CA	GLY		86	17.130	3.834	36.018	1.00		С	
ATOM	573	С	GLY	Α	86	16.573	4.453	37.289	1.00	27.73	С	
MOTA	574	0	GLY		86	15.563	5.163	37.268	1.00		0	
ATOM	575	N	ASN		87	17.273	4.186	38.392	1.00		N	
ATOM	576	CA	ASN		87	16.864	4.603	39.726			C	
ATOM	577	C	ASN		87	17.849	5.602	40.320	1.00		C	
ATOM	578	0	ASN		87	17.932	5.762	41.539	1.00		0	
ATOM ATOM	579 580	CB	ASN		87		3.367	40.644	1.00		C	
ATOM .	580 581	N.CA	GLY GLY		88 88	18.601 19.528	6.273 7.307	39.455 39.888	1.00		N C	
ATOM	582	C	GLY		88	18.762	8.549	40.288	1.00		C	
ATOM	583	0	GLY		88	17.570	8.654	40.001	1.00		ō	
ATOM	584	N	ASP		89	19.437	9.489	40.945	1.00		N	
ATOM	585	CA	ASP		89	18.808	10.739	41.366	1.00		C	
ATOM	586	С	ASP		89	18.761	11.755	40.227	1.00	26.69	С	
ATOM	587	0	ASP	A	89	19.697	11.848	39.446	1.00		0	
MOTA	588	CB	ASP	A	89	19.596	11.372	42.504	1.00	26.95	С	
MOTA	589	CG	ASP	A	89	19.375	10.688	43.834		27.28	C	
MOTA	590		ASP		89	18.499	9.811	43.939		29.31	0	
MOTA	591		ASP		89	20.040	10.983	44.839		27.32	0	
ATOM	592	N	PHE		90	17.687	12.531	40.152		26.24	N	
MOTA	593	CA C	PHE		90	17.598	13.594	39.165		26.10 26.23	C	
MOTA MOTA	. 594 595	0	PHE		90 90	17.407 16.629	14.931 15.037	39.866 40.811		26.48	0	
ATOM	596	СВ	PHE		90	16.460	13.322	38.184		25.91	Ċ	
ATOM	597	CG	PHE		90	16.747	12.201	37.241		25.26	d	
ATOM	598		PHE		90	16.601	10.886	37.640		25.32	d	
ATOM	599		PHE		90	17.190	12.459	35.958		26.02	C	
MOTA	600	CE1	PHE	Α	90	16.872	9.856	36.777	1.00	24.09	C	;
MOTA	601		PHE		90	17.460	11.427	35.091		25.07	C	
MOTA	602		PHE		90		10.117			24.67	C	;
MOTA	603	N	SER		91	18.149	15.941	39.430		26.33	N	
ATOM	604	CA	SER		91	17.985	17.280	39.973		26.48	C	
ATOM	605	C	SER		91	16.777	17.923	39.310		26.71	C	
MOTA	606 607	O	SER		91	16.696	18.029	38.077 39.763		26.09 26.25	. 0	
ATOM ATOM	608	CB OG	SER SER		91 91	19.226 20.364	18.152 17.543	40.326		26.25	C	
ATOM	609	N	VAL		92	15.835	18.327	40.150		27.06	N	
ATOM	610	CA	VÄL		92	14.629	18.971	39.695		27.44	C	
ATOM	611	C	VAL		92	14.468	20.295	40.405		27.57	Č	
ATOM	612	0	VAL		92	14.475	20.376	41.642		26.69	C	
ATOM	613	СВ	VAL		92	13.407	18.132	40.004		27.60	C	
MOTA	614		VAL		92	12.164	18.800	39.432		28.15	C	
ATOM	615		VAL		92	13.584	16.731	39.457		27.84	C	2
ATOM	616	N	TYR		93	14.312	21.334	39.598		27.77	I.	
ATOM	617	CA	TYR		93	14.120	22.661	40.108		27.91	C	
ATOM	618	C	TYR		93	12.654	22.940	40.172		28.16	C	
ATOM	619	O	TYR		93	11.894	22.525	39.303		28.02	C	
MOTA MOTA	620 621	CB CG	TYR TYR		93 93	14.810 16.291	23.673 23.593	39.216 39.368		27.94 29.53	C	
AT ON	021	CG	TIK	· A	73	10.231	23.333	39.300	1.00	29.53	(•

ATOM	622	CD1	TYR A		93	16.929	24.258	40.395	1.00 29.48	С
ATOM	623	CD2	TYR A		93	17.046	22.815	38.522	1.00 30.95	С
ATOM	624	CE1	TYR A	1	93	18.266	24.169	40.553	1.00 29.93	С
MOTA	625	CE2	TYR A	1	93	18.386	22.726	38.679	1.00 31.90	С
MOTA	626	CZ	TYR A	1	93	18.985	23.402	39.704	1.00 31.56	С
ATOM	627	ОН	TYR A	1	93	20.327	23.306	39.878	1.00 35.47	0
ATOM	628		SER A		94	12.282	23.669	41.208	1.00 28.70	N
ATOM	629		SER A		94	10.913	24.037	41.459	1.00 29.47	C
ATOM	630	C	SER A		94	10.856	25.547	41.554	1.00 29.69	С
ATOM	631	Ō	SER A		94	11.705	26.167	42.187	1.00 29.50	0
MOTA	632	СВ	SER A		94	10.456	.23.411	42.774	1.00 29.32	C
ATOM	633	OG	SER A		94	9.093	23.701	43.009	1.00 30.85	0
ATOM	634		ALA A		95	9.858	26.146	40.928	1.00 30.39	И
ATOM	635	CA	ALA A		95	9.760	27.591	40.929	1.00 31.04	С
ATOM	636	C	ALA A		95	8.330	28.064	40.932		С
ATOM	637	ō	ALA I		95	7.425	27.386	40.452	1.00 31.87	0
ATOM	638	СВ	ALA Z		95	10.480	28.165	39.716	1.00 31.12	C
MOTA	639	N	SER I		96	8.147	29.258	41.467	1.00 32.54	N
MOTA	640	CA	SER A		96	6.848	29.891	41.489	1.00 33.42	C
MOTA	641	C	SER A		96	6.708	30.869	40.326	1.00 33.15	Č
MOTA	642	Ö	SER .		96	5.662	31.487	40.163	1.00 34.35	Ō
MOTA	643	СВ	SER :		96	6.673	30.661	42.787	1.00 33.88	Č
ATOM	644	OG	SER .		96	5.380	31.217	42.815	1.00 35.79	Ō
ATOM	645	И	THR		97	7.775	31.031	39.554	1.00 32.09	N
ATOM	646	CA	THR		97	7.797	31.920	38.397	1.00 31.44	Ċ
MOTA	647	C	THR		97	8.185	31.095	37.191	1.00 30.26	· c
ATOM	648	Ö	THR		97	8.693	30.003	37.348	1.00 29.72	. 0
ATOM	649	СВ	THR		97	8.857	33.031	38.582	1.00 31.64	Ċ
ATOM	650	OG1			97	9.147	33.656	37.323	1.00 32.17	ō
	651	CG2	THR		97	10.227	32.455	38.978	1.00 31.73	C
MOTA			HIS		98	7.974	31.623	35.996	1.00 29.35	Ŋ
MOTA	652 653	N CA	HIS		98	8.379	30.915	34.780	1.00 28.83	C
ATOM			HIS		98	9.899	30.969	34.789	1.00 28.37	Č
ATOM	654 655	С 0	HIS		98	10.467	30.189	33.824	1.00 27.53	ō
ATOM ATOM	. 656	CB	HIS		98	7.671	31.490	33.548	1.00 28.76	Č
ATOM	657	CG	HIS		98	7.936	32.942	33.309	1.00 28.53	Č
	658		HIS		98	7.271	33.944	33.984	1.00 29.18	N
ATOM	659		HIS		98	8.793	33.566	32.463	1.00 29.68	C
ATOM			HIS		98	7.708	35.120	33.568	1.00 29.42	c
ATOM	660 661		HIS		98	8.638	34.919	32.650	1.00 29.10	N
ATOM	662	NEZ	LYS		99	10.562	31.874	35.299	1.00 27.85	N
ATOM ATOM	663	CA			99	11.997	32.041	35.124		C
	664				99	12.878	31.143	35.124	1.00 27.69	c
ATOM ATOM	665	С 0	LYS LYS		99	12.892	31.278	37.216	1.00 29.10	ō
	666		LYS		99	12.366	33.498	35.349	1.00 28.47	Ċ
ATOM ATOM	667	CB CG	LYS		99	11.836	34.410	34.255	1.00 30.42	· c
	668		LYS		99	12.431	35.791	34.347	1.00 30.42	, .C
MOTA	669	CD			99	11.757	36.624	35.421	1.00 34.45	C
MOTA		CE	LYS			10.569		34.884	1.00 34.43	N
MOTA	670	NZ	LYS		99.	13.621	30.237	35.376	1.00 35.35	N
ATOM	671	N	PHE					36.127	1.00 25.95	C
ATOM	672	CA	PHE			14.551				C
MOTA	673	C	PHE			15.978		35.995	1.00 25.87	
ATOM	674	0	PHE			16.809		35.247	1.00 25.86 1.00 25.48	0 C
ATOM	675	CB	PHE			14.469		35.686		
ATOM	676	CG	PHE				· 27.267	36.109		C
MOTA	677		PHE			12.047		35.388		C
ATOM	678		PHE			13.191		37.238	1.00 25.18	C
ATOM	679		PHE			10.886		35.772		C
ATOM	680		PHE			12.030		37.631	1.00 25.79	
MOTA	681	CZ			100	10.878		36.898		C
MOTA	682	N	LEU	A	101	16.237	30.997	36.709	1.00 25.77	N

MOTA	683	CA	LEU A 103	17.549	31.589	36.747	1.00 25.85	С
MOTA	· 684	С	LEU A 10	. 18.527	30.605	37.381	1.00 25.87	С
MOTA	685		LEU A 10:	18.319	30.136	38.503	1.00 24.99	0
ATOM	686	СВ	LEU A 10	17.488	32.876	37.559	1.00 25.84	С
ATOM	687		LEU A 10		33.656	37.708	1.00 26.07	С
ATOM	688		LEU A 10		34.200	36.377	1.00 25.11	Ċ
ATOM	689		LEU A 10		34.800	38.710	1.00 27.75	Ċ
ATOM	690	N	TYR A 10		30.274	36.644	1.00 26.56	N
ATOM	691	CA	TYR A 10		29.380	37.159	1.00 26.99	Ċ
ATOM	692	C	TYR A 10		30.072	38.260	1.00 27.10	č
ATOM	693	Õ	TYR A 10		31.264	38.174	1.00 27.00	ō
ATOM	694	CB	TYR A 10		28.939	36.053	1.00 27.26	· c
ATOM	695	CG	TYR A 10		28.088	36.620	1.00 28.93	C
ATOM	696	CD1	TYR A 10		26.750	36.914	1.00 29.52	Č
ATOM	697	CD2	TYR A 10		28.636	36.909	1.00 23.32	Ċ
ATOM	698	CE1	TYR A 10		25.979	37.480	1.00 32.23	C
ATOM	699	CE2	TYR A 10		27.872	37.470	1.00 32.23	c
								. c
ATOM	700	CZ	TYR A 10		26.549	37.750	1.00 33.88	
ATÓM	701	ОН	TYR A 10		25.794	38.314	1.00 38.68	0
ATOM	702	N	TYR A 10	_	29.322	39.296	1.00 26.83	N
ATOM	703	CA	TYR A 10		29.840	40.343	1.00 27.22	. C
ATOM	704	C	TYR A 10		28.750	40.834	1.00 26.77	C
MOTA	705	0	TYR A 10		27.556	40.853	1.00 25.60	0
MOTA	706	CB	TYR A 10		30.440	41.517	1.00 27.38	C
ATOM	707	CG	TYR A 10		29.493	42.154	1.00 29.11	C
ATOM	708	CD1			29.340	41.639	1.00 30.58	C
ATOM	709		TYR A 10		28.759	43.279	1.00 32.13	C
ATOM	710	CE1	TYR A 10		28.469	42.212	1.00 32.78	C
MOTA	711	CE2			27.887	43.877		. C
MOTA	712	CZ	TYR A 10		27.745	43.329	1.00 34.41	C
MOTA	713	OH	TYR A 10		26.888	43.892	1.00 37.44	0
ATOM	714	N	ASP A 10		29.182	41.225	1.00 26.36	N
ATOM	715	CA	ASP A 10		28.273	41.673	1.00 26.28	С
MOTA	716	С	ASP A 10		28.239	43.184	1.00 26.21	C
MOTA	717	0	ASP A 10		29.212	43.845	1.00 25.45	0
MOTA	718	CB	ASP A 10		28.765	41.154	1.00 25.92	С
ATOM	719	CG	ASP A 10	4 28.330	27.889	41.575	1.00 27.39	С
ATOM	720	OD1	ASP A 10	4 28.161	26.973	42.437	1.00 27.13	0
MOTA	721	OD2	ASP A 10		28.068	41.075	1.00 27.68	0
ATOM	722	N	GLU A 10		27.114	43.724	1.00 26.46	N
MOTA	723	CA	GLU A 10	5 25.218	26.962	45.162	1.00 27.02	C
ATOM	724	С	GLU A 10	5 26.540	27.199	45.916	1.00 26.91	С
MOTA	725	0	GLU A 10	5 26.523	27.718	47.026	1.00 26.51	0
ATOM	726	CB	GLU A 10	24.602	25.587	45.481	1.00 27.45	C
ATOM	727	CG	GLU A 1	23.088	25.556	45.254	1.00 29.46	С
ATOM	728	CD	GLU A 1	22.527	24.158	45.025	1.00 32.85	С
ATOM	729	OE1	GLU A 10	22.908	23.234	45.765	1.00 32.90	0
ATOM	730	OE2	GLU A 1	21.703	23.980	44.085	1.00 35.16	0
ATOM	731	N	LYS A 1	27.680	26.874	45.305	1.00 27.12	N
MOTA	732	CA	LYS A 1			45.983	1.00 27.54	С
MOTA	733	С	LYS A 1			46.258	1.00 27.70	С
MOTA	734	0	LYS A 1			47.099	1.00 27.61	0
ATOM	735	CB	LYS A 1			45.163	1.00 27.58	С
ATOM	736	CG	LYS A 1			44.918	1.00 28.61	
ATOM	737	N	LYS A 1			45.537	1.00 27.99	N
ATOM	738	CA	LYS A 1			45.694	1.00 28.30	C
MOTA	739	C	LYS A 1			46.631	1.00 29.21	Č
ATOM	740	Ö	LYS A 1			46.917	1.00 29.08	ő
MOTA	741	СВ	LYS A 1			44.324	1.00 28.30	C
ATOM	742	CG	LYS A 1			43.516		C
ATOM	743	CD	LYS A 1			42.034		C
	, 10	-55	AL L				2.00 27.23	

ATOM	744		LYS A		31.584	31.518	41.315		26.86		С
MOTA			LYS A		31.642	31.889	39.870		24.80		N
MOTA	746		MET A		27.041	30.781	47.125		30.08		N
ATOM	747			1 108	26.031	31.405	47.982		31.53		C
ATOM	748		MET A		26.581	31.952	49.309		32.44		C
MOTA	749		MET A		26.102	32.972	49.812		32.47		0
MOTA	750		MET A		24.862	30.452	48.218		31.81		С
ATOM	751		MET A		24.072	30.193	46.932		33.07 35.76		C S
ATOM	752			A 108	22.625	29.140	47.064 48.050		35.76		C
ATOM ATOM	753 754			A 108 A 109	21.540 27.603	30.140 31.315	49.860		33.56		N
ATOM	755			A 109	28.154	31.769	51.138		34.94		C
ATOM	756			A 109	28.651	33.212	51.060		35.81		Ċ
ATOM	757			A 109	28.483	33.989	51.991		36.23		Ö
ATOM	758	СВ		A 109	29.279	30.838	51.606		34.82		C
ATOM	759	N		A 110	29.236	33.575	49.929		37.05		N
ATOM	760	CA		A 110	29.774	34.918	49.748		37.94		С
MOTA	761	С		A 110	28.731	35.992	49.413	1.00	38.13		С
ATOM	762	Ο.	ASN 2	A 110	29.064	37.167	49.293	1.00	37.92		o ·
MOTA	763	CB	ASN 2	A 110	30.855	34.878	48.669	1.00	38.16		С
MOTA	764	CG		A 110	32.050	34.035	49.079.		39.37		С
ATOM	765			A 110	32.407	33.964	50.265		40.12		0
MOTA	766			A 110	32.670	33.377	48.103		39.46		N
MOTA	767	N		A 111	. 27.480	35.588	49.234		38.71		N.
ATOM	768	CA		A 111	26.408		48.966		39.02		C
ATOM	769	C		A 111	25.180	36.135	49.773		39.71		C
ATOM	770	0		A 111	24.143	35.747	49.232 47.471		39.45 38.97		O C
ATOM	771 772	CB CG		A 111 A 111	26.091 27.110	36.603 37.362	46.672		38.04		C
ATOM ATOM	773			A 111	28.329	36.791	46.363		37.99		c
MOTA	774			A 111	26.851	38.642	46.235		36.83		C
MOTA	775			A 111	29.269	37.493	45.635		37.68		Ċ
ATOM	776			A 111	27.788	39.339	45.500		36.08		Ċ
MOTA	777	CZ		A 111	28.994	38.768	45.208	1.00	35.84		С
MOTA	778	N		A 112	25.315	36.267	51.085	1.00	40.62		N
MOTA	779	CA	GLN	A 112	24.286°	35.852	52.029	1.00	41.31	-	С
ATOM	780	C	GLN	A 112	22.915	36.430	51.721	1.00	41.10		С
MOTA	781	0		A 112	21.906	35.827	52.060		41.31		0
MOTA	782	CB		A 112	24.701	36.236	53.451		41.65		С
MOTA	783	CG		A 112	26.058	35.694	53.882		43.80		C
ATOM	784	CD		A 112	26.104	34.177	53.938		46.42		Ċ
MOTA	785			A 112	25.394	33.501	53.191		48.56		0
ATOM	786			A 112	26.951	33.637	54.816 51.074		46.94	-	N
ATOM	787 788	N CA		A 113	22.876 21.606	37.588 38.229	50.749		41.02		N C
MOTA MOTA	789	CA		A 113 A 113	20.954	37.760	49.440		40.71		C
ATOM	790	Ö		A 113	19.889	38.251	49.071		40.77		Ö
ATOM	791	СВ		A 113	21.778	39.753	50.737		41.09		Ċ
ATOM	792	CG		A 113	22.129	40.314	52.123		41.51		Č
MOTA	793			A 113	21.717	39.772	53.158		40.60		O
ATOM	794			A 113	22.892	41.401	52.141	1.00	41.19		N
ATOM	795	N		A 114	21.571	36.826	. 48.725	1.00	40.34		N
MOTA	796	CA		A 114	20.934	36.321	47.515	1.00	39.86		С
MOTA	797	С		A 114	19.908	35,266			39.46		С
MOTA	798	0		A 114	20.235	34.299			38.82		0
MOTA	799	CB		A 114	21.940	35.714	46.552		39.96		С
MOTA	800	CG		A 114	21.298	35.059			40.54		C
ATOM	801			A 114	20.670	35.828			40.29		С
ATOM	802			A 114	21.295	33.679			40.62		C
ATOM	803			A 114	20.061	35.237			40.20		C
MOTA	804	CEZ	PHE	A 114	20.684	33.082	44.126	1.00	40.36		C

ATOM	805 CZ	PHE A 114	20.066	33.866	43.172	1.00 40.52
ATOM .	806 N	LYS A 115	18.669	35.457	47.461	1.00 39.11
ATOM	807 CA	LYS A 115	17.596	34.529	47.787	1.00 39.02
ATOM	808 C	LYS A 115	17.042	33.938	46.497	1.00 38.71
ATOM	809 0	LYS A 115	16.285	34.590	45.787	1.00 39.00
ATOM	810 CB	LYS A 115		35.251	48.578	1.00 39.14
ATOM	811 N	PRO A 116		32.691	46.213	1.00 38.17
ATOM	812 CA	PRO A 116	17.027	32.060	44.938	1.00 37.95
	813 C	PRO A 116	15.532	31.889	44.783	1.00 37.38
ATOM	813 C	PRO A 116	14.865	31.506	45.733	1.00 37.36
ATOM		PRO A 116		30.679	45.004	1.00 38.15
ATOM	815 · CB			30.604	46.297	1.00 38.40
ATOM	816 CG	PRO A 116	18.416			1.00 38.19
ATOM	817 CD	PRO A 116	18.079	31.775	47.125	
MOTA	818 N	ARG A 117		32.161	43.590	1.00 36.84
MOTA	819 CA	ARG A 117		32.028	43.293	1.00 36.61
ATOM	820 C	ARG A 117		30.581	42.984	1.00 36.38
MOTA	821 O	ARG A 117		30.230	42.913	1.00 36.44
MOTA	822 CB	ARG A 117	13.235	32.913	42.122	1.00 36.62
ATOM	823 N	SER A 118		29.745	42.777	1.00 35.79
MOTA	824 CA	SER A 118	14.025	28.339		1.00 35.51
MOTA	825 C	SER A 118	14.844	27.491		1.00 35.35
MOTA	826 O	SER A 118	15.888	27.923	43.991	1.00 35.16
ATOM	827 CB		14.330	27.976	41.086	1.00 35.26
ATOM	828 OG		15.689	28.164	40.795	1.00 35.14
ATOM	829 N	ASN A 119		26.306		1.00 35.11
ATOM	830 CA					1.00 35.21
ATOM	831 C	ASN A 119	15.233			1.00 34.26
ATOM	832 0	ASN A 119	14.401			1.00 34.11
ATOM	833 CB		14.145			1.00 35.95
	834 CG		13.636			1.00 38.47
ATOM			14.417		47.025	1.00 41.76
ATOM		1 ASN A 119		26.511	46.657	1.00 42.21
MOTA		2 ASN A 119	12.314	23.434	44.326	1.00 42.21
MOTA	837 N	ARG A 120	16.368			1.00 33.73
MOTA	838 CA		16.750	22.149		1.00 33.33
ATOM	839 C	ARG A 120	16.327			
MOTA	840 O	ARG A 120	16.523	21.138		1.00 33.07
MOTA	·841 CE		18.270	22.075		1.00 33.37
MOTA	842 CG	ARG A 120	18.759	20.889		1.00 32.70
MOTA	843 CI		20.277			1.00 31.64
MOTA	844 NE		20.892			1.00 31.16
MOTA	845 C2		21.233	20.357	44.993	1.00 31.33
MOTA	846 N	11 ARG A 120	21.027			
MOTA	847 N	12 ARG A 120	21.789	20.867	46.077	1.00 31.01
MOTA	848 N	GLU A 121	15.735	20.001	44.137	1.00 32.98
MOTA	849 C	A GLU A 121	15.379	18.827	44.904	1.00 32.85
MOTA	850 C	GLU A 121	15.846	17.630	44.095	1.00 32.17
ATOM	851 0	GLU A 121	15.744	17.612	42.864	1.00 32.36
ATOM	852 CI	B GLU A 121.	13.874	18.767	45.179	1.00 33.21
ATOM	853 C	G GLU A 121	13.420	17.468	45.826	1.00 35.39
ATOM	854 CI		12.189	17.629	46.699	1.00 38.11
ATOM		E1 GLU A 121	12.326	18.152	47.830	1.00 41.26
ATOM		E2 GLU A 121	11.091			1.00 39.55
MOTA	857 N		16.400	16.648		1.00 31.28
MOTA	858 C		16.886			1.00 30.61
ATOM	859 C		15.814	14.392		1.00 30.31
ATOM	860 O		15.328			1.00 30.07
ATOM		B GLU A 122	18.163			1.00 30.52
		G GLU A 122	19.293			1.00 29.67
ATOM		D GLU A 122	19.747			
MOTA		E1 GLU A 122	20.120			
MOTA			19.734			
MOTA	865 O	E2 GLU A 122	19./34	11.433	76.314	1.00 27.95

MOTA	866	N	MET 2	A	123	15.432	13.751	43.202	1.00 29.74	N
MOTA	867	CA			123	14.407	12.728	43.277	1.00 29.77	С
MOTA	868				123	14.594	11.683	42.202	1.00 29.31	С
ATOM	869	0	MET :			15.408	11.842	41.294	1.00 29.42	0
ATOM	870	CB			123	13.016	13.354	43.165	1.00 29.81	C
MOTA	871	CG	MET .			12.749	14.057	41.865	1.00 30.27	C
ATOM ATOM	872 873	SD CE	MET .			11.181 11.582	14.960 16.371	41.871 42.804	1.00 31.65 1.00 31.47	s C
ATOM	874	N	LYS .			13.835	10.604	42.332	1.00 31.47	N
ATOM	875	CA	LYS			13.841	9.535	41.352	1.00 28.33	C
ATOM	876	C	LYS			12.959	9.976	40.191	1.00 27.51	Č
ATOM	877	0	LYS .			12.077	10.817	40.361	1.00 26.52	0
ATOM	878	CB	LYS .			13.330	8.242	41.984	1.00 28.45	С
MOTA	879	CG	LYS .			14.153	7.783	43.204	1.00 29.42	С
MOTA	880	CD	LYS			15.597	7.442	42.804	1.00 30.46	С
ATOM	881	CE	LYS			16.479	7.067	43.992	1.00 30.52	С
MOTA	882	NZ	LYS			17.928	. 7.324	43.699	1.00 30.05	N
ATOM ATOM	883 884	N CA	PHE		125	13.188 12.477	9.407 9.871	39.014	1.00 26.98	N
ATOM	885	CA	PHE			10.974	9.871	37.826 37.972	1.00 26.83 1.00 26.77	C
ATOM	886	0	PHE			10.245	10.673	37.585	1.00 26.77	0
ATOM	887	СВ	PHE			12.927	9.138	36.568	1.00 26.71	Č
ATOM	888	CG	PHE			12.613	9.891	35.316	1.00 26.32	Ċ
ATOM	889.	CD1				13.476	10.876	34.849	1.00 26.29	C
MOTA	890		PHE			11.438	9.657	34.635	1.00 26.06	C
ATOM	891	CE1	PHE	A	125	13.183	11.594	33.715	1.00 25.70	С
ATOM	892	CE2	PHE			11.140	10.368	33.483	1.00 26.70	С
ATOM	893	CZ	PHE			12.018	11.341	[.] 33.025	1.00 26.87	С
ATOM	894	N	HIS			10.527	8.649	38.550	1.00 26.77	N
ATOM	895	CA	HIS			9.113	8.396	38.753	1.00 26.82	C
ATOM	896	С	HIS			8.517	9.390	39.734	1.00 26.68	C
ATOM ATOM	897	O	HIS			7.326	9.670	39.687	1.00 26.03	0
ATOM	898 899	CB CG	HIS HIS			8.882 9.028	6.951 6.767	39.238 40.717	1.00 27.07 1.00 27.39	C
ATOM	900		HIS			7.959	6.836	41.582	1.00 27.39	N
ATOM	901		HIS			10.115	6.505	41.484	1.00 28.33	· C
ATOM	902		HIS			8.382	6.636	42.819	1.00 28.68	C
ATOM	903		HIS			9.687	6.439	42.788	1.00 27.97	Ŋ
MOTA	904	N	GLU			9.342	9.918	40.630	1.00 27.00	N
ATOM	905	CA	GLU	A	127	8.876	10.930	41.572	1.00 27.34	С
ATOM	906	С	GLU	_		8.683	12.259	40.838	1.00 27.36	C
ATOM	907	0	GLU			7.761	13.026	41.126	1.00 26.86	0
MOTA	908	CB	GLU			9.862	11.084	42.728	1.00 27.31	С
ATOM	909	CG	GLU			10.018	9.821	43.552	1.00 28.69	C
ATOM ATOM	910 911	CD	GLU			10.959	9.992	44.722	1.00 29.65	С
ATOM ·	912		GLU GLU			12.139 10.509	10.318 9.787	44.485 45.876	1.00 29.56 1.00 30.92	0
ATOM	913	N			128	9.554	12.519	39.876	1.00 30.92	O N
ATOM	914	CA			128	9.453	13.736	39.068	1.00 27.31	C
ATOM	915	C			128	8.149	13.658	38.282	1.00 29.04	c
ATOM	916	0			128	7.354	14.600	38.255	1.00 29.03	ō
ATOM	917	СВ			128	10.643	13.838	38.115	1.00 27.74	Ċ
MOTA	918	CG			128	10.427	14.792	36.959	1.00 27.06	С
ATOM	919		PHE			10.189	16.138	37.185	1.00 25.41	С
ATOM	920		PHE			10.480	14.343	35.657	1.00 25.60	С
MOTA	921		PHE			9.985	17.000	36.144	1.00 25.41	С
MOTA	922		PHE			10.281	15.215	34.604	1.00 26.59	C
MOTA	923	CZ			128	10.032	16.540	34.846	1.00 25.61	C
MOTA	924	N			129	7.925	12.500	37.677	1.00 29.90	N
MOTA	925	CA C			129	6.756	12.285	36.847	1.00 30.82	c
MOTA	926	C	٧AL	A	129	5.476	12.447	37.669	1.00 31.61	С

ATOM	927	0	VAL	Α	129	4.515	13.091	37.234	1.00 31.39		0
ATOM	928	CB	VAL	Α	129	6.793	10.883	36.213	1.00 30.92		Č
ATOM	929	CG1	VAL	Α	129	5.479	10.582	35.503	1.00 31.15		
ATOM	930		VAL			7.975	10.751	35.253			C
ATOM	931	N			130				1.00 30.61		С
ATOM	932					5.475	11.858	38.861	1.00 32.42		N
		CA			130	4.332	11.946	39.761	1.00 33.13		C
ATOM	933	С			130	4.070	13.403	40.126	1.00 33.42		С
ATOM	934	0	GLU	A	130	2.930	13.867	40.081	1.00 33.01		ō
ATOM	935	CB	GLU	Α	130	4.587	11.108	41.017	1.00 33.20		Č
ATOM	936	CG			130	4.537	9:609	40.755	1.00 33.20		
ATOM	937	CD			130	5.294	8.792	41.789			C
ATOM	938		GLÜ	7	130				1.00 35.55		·C
MOTA	939	OES	CLU	77	120	5.630	9.339	42.861	1.00 37.02		0
			GLU			5.558	7.598	41.525	1.00 35.99		0
ATOM	940	N			131	5.128	14.120	40.486	1.00 34.00		N
ATOM	941	CA			131	4.994	15.538	40.800	1.00 34.79		С
ATOM	942	С	LYS	Α	131	4.354	16.286	39.637	1.00 35.25		c
ATOM	943	0	LYS	Α	131	3.449	17.089	39.835	1.00 34.81		. 0
ATOM	944	CB	LYS			6.345	16.171	41.100	1.00 34.89		
MOTA	945	CG			131	6.597	16.477				C
ATOM	946	CD	LYS			7.191		42.554	1.00 35.57		C
ATOM	947	CE				·	17.868	42.694	1.00 36.25		C
			LYS			7.862	18.072	44.034			С
ATOM	948	NZ	LYS			8.108	19.526	44.332	1.00 37.49		N
ATOM	949	N	LEU			4.829	16.038	38.422	1.00 36.00		N
MOTA	950	CA	LEU			4.243	16.701	37.268	1.00 37.05		C
ATOM	951	С	LEU	A	132	2.755	16.406	37.170	1.00 37.67		Č
ATOM	952	0	LEU			1.963	17.300	36.870	1.00 37.77		
ATOM	953	СВ	LEU			4.919	16.260	35.979			0
ATOM	954	CG	LEU			6.310			1.00 37.39		С
ATOM	955		LEU				16.803	35.710	1.00 38.29		С
ATOM	956					6.783	16.289	34.363	1.00 39.35		C
			LEU			6.306	18.314	35.721	1.00 39.70		С
ATOM	957	N	GLN	Α	133	2.386	15.151	37.417	1.00 38.34		· N
ATOM	958	CA	${\tt GLN}$			0.989	14.730	37.373	1.00 39.11		C
ATOM	959	С	GLN	A	133	0.132	15.434	38.427	1.00 39.73	•	Č
ATOM	960	0	GLN	Α	133	-0.966	15,897	38.126	1.00 39.61		
ATOM	961	CB	GLN			0.886	13.213	37.538	1.00 39.01		0
ATOM	962	N	ASP			0.629	15.507				С
ATOM	963	CA	ASP					39.658	1.00 40.61	•	N
ATOM	964	C				-0.108	16.149	40.747	1.00 41.70		C
			ASP			-0.398	17.626	40.451	1.00 41.68		С
ATOM	965	0	ASP			-1.470	18.137	40.770	1.00 41.28		0
ATOM	966	CB	ASP			0.678	16.030	42.056	1.00 42.32		C
ATOM	967	CG	ASP	A	134	-0.165	16.351	43.286	1.00 44.92		Č
ATOM	968	OD1	ASP	Α	134	-1.235	16.991	43.152			ŏ
MOTA	969	OD2	ASP	Α	134	0.164	15.991	44.442	1.00 48.64		
MOTA	970	N	ILE			0.563	18.312	39.842	1.00 41.92		0
ATOM	971	CA	ILE			0.383	19.717				· N
ATOM	972	C	ILE			-0.715		39.512	1.00 42.18		С
ATOM	973	ō	ILE			,	19.862	38.471	1.00 42.41		С
						-1.635	20.664	38.634	1.00 42.49		0
ATOM	974	CB			135		20.324	38.997	1.00 42.17		С
MOTA	975		ILE			2.720	20.399	40.131	1.00 42.25		С
MOTA	976	CG2	ILE	A	135	1.451	21.708	38.437	1.00 42.11		c
MOTA	977	CD1	ILE	Α	135	4.151	20.438	39.653	1.00 42.91		Č
ATOM	978	N	GLN			-0.614	19.075	37.407	1.00 42.71		
ATOM	979	CA	GLN			-1.593	19.114				N
ATOM	980	С	GLN					36.333	1.00 43.09		C
ATOM	981	Ö				-2.991	18.935	36.900	1.00 43.56		С
ATOM	982		GLN			-3.863	19.785	36.707	1.00 43.93		0
		СВ	GLN			-1.298	18.031	35.317	1.00 43.10		С
ATOM	983	N	GLN			-3.181	17.844	37.635	1.00 43.82		N
ATOM	984	CA	GLN			-4.486	17.493	38.182	1.00 44.02		Ċ
ATOM	985	С	GLN	A	137	-5.023	18.540	39.144	1.00 44.08		c
ATOM	986	0	GLN	A	137	-6.202	18.891	39.080	1.00 44.46		
ATOM	987	CB	GLN	Α	137	-4.425	16.124	38.868	1.00 44.00		0
								55.000	±.00 44.00		С

ATOM	988 N	ARG A 138	-4.169	19.043	40.031	1.00 43.93	N
ATOM	989 CA	ARG A 138				1.00 43.76	C
ATOM	990 C	ARG A 138		_ :		1.00 43.34	C
ATOM	991 0	ARG A 138		_		1.00 43.54	0
ATOM	992 CB	ARG A 138				1.00 43.84	C
ATOM	993 CG					1.00 44.85	C C
MOTA	994 CD			20.279		1.00 45.82	N
MOTA	995 NE			21.197		1.00 46.44	C
MOTA	996 CZ			20.863		1.00 47.95 1.00 49.02	N
MOTA		1 ARG A 138		19.627		1.00 47.70	N
MOTA		2 ARG A 138	1.864	21.767		1.00 47.70	N
MOTA	999 ห	GLY A 139	-4.450	21.569 22.871		1.00 42.02	C
MOTA	1000 CA		-4.371	23.820	39.174	1.00 41.28	
MOTA	1001 C	GLY A 139	-3.389	25.030	39.174	1.00 41.58	o
MOTA	1002 0	GLY A 139	-3.607 -2.291	23.292	39.703	1.00 40.31	, N
ATOM	1003 N	GLY A 140	-1.329	24.119	40.410	1.00 39.43	· c
ATOM	1004 CA		-0.563	25.070	39.512	1.00 38.71	C
MOTA	1005 C	GLY A 140	-0.495	24.871	38.294	1.00 38.40	C
MOTA	1006 O		0.003	26.117	40.110	1.00 37.82	N
MOTA	1007 N		0.829	27.066	39.363	1.00 37.20	C
ATOM	1008 C		2.320	26.726	39.491	1.00 35.94	(
ATOM	1009 C 1010 O		3.160	27.356	38.845	1.00 35.76	(
MOTA			0.590	28.510	39.828	1.00 37.63	(
MOTA			-0.729	29.146	39.379	1.00 39.51	(
MOTA	1012 C		-0.936	29.164	37.866	1.00 41.63	(
MOTA		E1 GLU A 141	0.056	29.147	37.102	1.00 42.42	
MOTA		E2 GLU A 141	-2.115	29.202	37.434	1.00 43.77	(
MOTA	1015 O		2.652	25.742	40.326	1.00 34.29	1
MOTA MOTA		A GLU A 142	4.045	25.351	40.510	1.00 33.08	
MOTA	1017 C		4.655	24.938	39.170	1.00 31.87	
ATOM	1010 0		3.958	24.443	38.296	1.00 31.87	
MOTA		B GLU A 142	4.170	24.201	41.519	1.00 32.96	
ATOM		G GLU A 142	5.610	23.914	41.942	1.00 32.71	
ATOM		D GLU A 142	5.761	22.730	42.896	1.00 33.55	
ATOM		E1 GLU A 142	4.778	22.001	43.146	1.00 32.41	
ATOM		E2 GLU A 142	6.888	22.520		1.00 34.13	
MOTA		ARG A 143	5.954	25.156		1.00 30.56	
MOTA		CA ARG A 143	6.662	24.766		1.00 29.79	
ATOM		ARG A 143	7.878	23.939		1.00 28.70	
MOTA	1028) ARG A 143	8.565	24.210		1.00 28.88	
MOTA	1029	CB ARG A 143	7.142	25.991		1.00 29.90	
MOTA	1030	CG ARG A 143	6.043	26.832		1.00 30.80	
MOTA		CD ARG A 143	6.591	27.992		1.00 30.70	
MOTA		NE ARG A 143	5.538	28.715		1.00 30.86 1.00 29.53	
MOTA		CZ ARG A 143	5.168	28.487		1.00 27.51	
ATOM		NH1 ARG A 143	5.763			1.00 27.31	
MOTA		NH2 ARG A 143	4.196			1.00 30.04	
MOTA		N LEU A 144	8.156			1.00 27.27	,
MOTA		CA LEU A 144	9.319				
. ATOM		C LEU A 144					
MOTA		O LEU A 144	9.755 8.893				
ATOM		CB LEU A 144	7.922				
ATOM		CG LEU A 144	7.575				
ATOM		CD1 LEU A 144 CD2 LEU A 144	8.488				
MOTA			11.511				•
MOTA		N TYR A 145 CA TYR A 145	12.458				
MOTA			13.516				
MOTA	1046	C TYR A 145 O TYR A 145	14.328				
MOTA	1047	CB TYR A 145	13.080				
MOTA	1048	OD TIV W TAN	25.500				

MOTA	1049	CG	TYR	A	145		13.522	23.419	33.666	1.00 21.34	С
MOTA	1050		TYR	Α	145		13.824	22.333	32.863	1.00 20.11	С
MOTA	1051		TYR				13.662	24.691	33.119	1.00 21.14	С
ATOM	1052		TYR				14.219	22.494	31.563	1.00 20.22	C
MOTA	1053		TYR				14.075	24.866	31.807	1.00 19.81	С
ATOM	1054	CZ	TYR			•	14.349	23.764	31.027	1.00 19.19	С
MOTA	1055	OH	TYR				14.736	23.903	29.699	1.00 18.36	0
ATOM	1056	N	LEU				13.461	19.666	35.287	1.00 22.75	N
ATOM	1057	CA	LEU				14.490	18.661	35.516	1.00 23.17	С
ATOM	1058	С	LEU				15.720	19.005	34.679	1.00 22.99	. C
ATOM	1059	0	LEU				15.604	19.264	33.490	1.00 22.81	0
ATOM	1060	CB	LEU				13.980	17.282	35.115	1.00 23.33	C
ATOM	1061	CG	LEU				14.992	16.141	35.274	1.00 24.98	C
ATOM	1062		LEU				14.276	14.846	35.622	1.00 24.56	С
ATOM	1063		LEU				15.849	15.946	34.016	1.00 26.13	C
ATOM ATOM	1064	N	GLN				16.891	18.983	35.299	1.00 23.05	N
ATOM	1065 1066	CA C	GLN				18.135	19.314	34.619	1.00 23.65	C
ATOM			GLN				19.158	18.394	35.231	1.00 23.86	C
	1067	0	GLN				19.573	18.597	36.364	1.00 24.61	0
ATOM ATOM	1068 1069	CB	GLN				18.516	20.793	34.821	1.00 23.53	C
ATOM	1009	CG CD	GLN GLN				17.386	21.770	34.461	1.00 24.34	. C
ATOM	1070	OE1					17.800	23.238	34.482	1.00 26.20	С
ATOM	1071		GLN GLN				17.034 18.979	24.114	34.035	1.00 29.67	0
ATOM	1072	NE2			148		19.542	23.514 17.369	34.988	1.00 21.33 1.00 24.35	N N
ATOM	1073	CA	GLN			'	20.393		34.485		
ATOM	1074	C			148		21.319	16.314 15.753	35.006 33.964	1.00 24.70	C
ATOM	1075	Ö			148		20.898	15.733	32.866	1.00 25.16 1.00 24.21	0
ATOM	1077	СВ			148		19.525	15.172	35.526		C
ATOM	1077	CG			148	•	20.317	13.172	35.953	1.00 24.97 1.00 25.54	C
MOTA	1079	CD			148		21.275		37.085	1.00 25.54	G
ATOM	1080		GLN				20.892	14.256 14.941	38.042	1.00 26.38	0
ATOM	1081		GLN				22.522	13.786	36.976	1.00 26.73	N
ATOM	1082	N			149		22.592	15.704	34.321	1.00 25.94	N
ATOM	1083	CA			149		23.603	15.134	33.466	1.00 23.34	C
ATOM	1084	C			149		23.369	13.632	33.324	1.00 27.29	· č
ATOM	1085	Ö			149	•	23.081	12.965	34.303	1.00 27.25	Õ
ATOM	1086	СВ			149		24.990	15.430	34.075	1.00 27.91	C
MOTA	1087				149		25.282	16.829	33.901	1.00 30.41	ő
ATOM	1088				149			14.776	33.276	1.00 30.12	Č
ATOM	1089	N			150		23.461	13.117	32.100	1.00 27.79	N
MOTA	1090	CA			150		23.321	11.690			Ċ
MOTA	1091	c [']			150		24.549	10.935	32.364	1.00 28.42	C
MOTA	1092	0			150		25.682	11.261	32.002	1.00 28:86	. 0
ATOM	1093	CB			150		23.194	11.435	30.326	1.00 28.08	С
MOTA	1094	CG	LEU	Α	150		21.929	11.937	29.622	1.00 28.70	С
ATOM	1095	CD1	LEU	Α	150		22.016	11.725	28.117	1.00 28.62	С
ATOM	1096		LEU				20.697	11.260	30.175	1.00 29.47	С
MOTA	1097	N	ASN	Α	151	•	24.332	9.928	33.203	1.00 28.58	N
MOTA	1098	CA	ASN	A	151		25.434	9.156	33.781	.1.00 28.79	C
ATOM	1099	С	ASN	Α	151		25.194	7.636	33.782	1.00 29.24	. С
MOTA	1100	0	ASN	Α	151		24.197	7.163	33.238	1.00 29.60	0
MOTA	1101	CB			151		25.657	9.631	35.208	1.00 28.77	C
MOTA	1102	CG			151		24.459	9.367	36.084	1.00 28.05	С
MOTA	1103				151		23.936	8.246	36.126	1.00 29.02	0
MOTA	1104	ND2			151		24.000	10.396	36.772	1.00 26.99	N
MOTA	1105	N			152		26.083	6.885	34.437	1.00 29.71	N
ATOM	1106	CA			152		26.039	5.410	34.448	1.00 30.06	С
MOTA	1107	С			152		24.850	4.733	35.075	1.00 29.51	С
ATOM	1108	0			152		24.771	3.503	35.026		0
MOTA	1109	CB	ASP	A	152		27.199	4.829	35.250	1:00 30.99	С

MOTA	1110		ASP A 15		.447		35.048	1.00		С
MOTA	1111		ASP A 15		. 636	6.071	33.918	1.00		0
MOTA	1112	OD2	ASP A 15		.274	5.719	35.960	1.00		0
MOTA	1113	N	THR A 15		.959	5.468	35.722	1.00		N
MOTA	1114	CA	THR A 15		.831	4.792	36.359	1.00		С
MOTA	1115	С	THR A 15		. 685	4.594	35.387	1.00		С
MOTA	1116	0	THR A 15		.730	3.909	35.712	1.00		0
ATOM	1117	·CB	THR A 15	3 22	.330	5.552	37.584	1.00	28.53	С
MOTA	1118	OG1	THR A 15	3 21	.833	6.836	37.193	1.00	28.91	0
MOTA	1119	CG2	THR A 15	3 23	.473	5.855	38.540	1.00		С
MOTA	1120	N	VAL A 15		.766	5.171	34.194	1.00		N
MOTA	1121	CA	VAL A 15		.671	4.996	33.246	1.00		С
MOTA	1122	C	VAL A 15	4 20	.583	3.531	32.895	1.00		С
MOTA	1123	0	VAL A 15	4 21	.592	2.832	32.923		27.36	0
MOTA	1124	CB	VAL A 15		.838	5.826	31.964		26.05	С
MOTA	1125	CG1	VAL A 15		.914	7.279	32.312		26.14	С
MOTA	1126	CG2	VAL A 15		.071	5.383	31.182		25.62	С
MOTA	1127	N	GLY A 15	5 19	.379	3.072	32.568		26.71	N.
ATOM	1128	CA	GLY A 15	5. 19	.147	1.674	32.252		26.42	c.
ATOM	1129	C.	GLY A 15	55 19	.531	1.266	30.840		26.67	С
MOTA	1130	Ο.	GLY A 15	5 19	.894	2,093	29.983		26.52	0.
MOTA	1131	N	ARG A 15	66 19	.390	-0.028	30.599		26.49	N
MOTA	1132	CA	ARG A 15	66 19	.811	-0.684	29.364		26.54	C
MOTA	1133	С	ARG A 15	66 19	.305	-0.053	28.068		25.95	C
MOTA	1134	0	ARG A 15	66 20	.089	0.194	27.160		26.26	0
MOTA	1135	CB	ARG A 15		.429	-2.165	29.418		26.28	С
MOTA	1136	N	LYS A 15	57 18	.004	0.175	27.964		25.43	N
MOTA	1137	CA	LYS A 15	57 17	.460	0.777	26.756		25.11	C
MOTA	1138	С	LYS A 15		.026	2.198	26.517		25,50	C
MOTA	1139	0	LYS A 15		.249	2.595	25.372		25.14	0
MOTA	1140	CB	LYS A 15		.927	0.796	26.809	1.00		C
MOTA	1141	CG	LYS A 1		.255	-0.572	26.516		24.25	С
MOTA	1142	N	ILE A 15		3.257	2.956	27.585		25.35	N
MOTA	1143	CA	ILE A 1		3.766	4.326	27.432		25.61	C
MOTA	1144	С	ILE A 1		205	4.250	26.971		25.76	C
MOTA	1145	0	ILE A 1		0.661	5.058	26.166		25.39	0
MOTA	1146	СВ	ILE A 1		3.662	5.107	28.740		25.41	C
MOTA	1147		L ILE A 1		7.202	5.245	29.162		25.92	C
MOTA	1148		2 ILE A 1		9.297	6.475	28.601		25.61	C
MOTA	1149		L ILE A 1		6.331	5.924	28.174		27.88	C
MOTA	1150		. VAL A 1		0.909		27.481		26.10	N
MOTA	1151	CA	VAL A 1		2.276	3.010	27.079		26.57	C
MOTA	1152	С	VAL A 1		2.279	2.703	25.585		26.40	С
MOTA	1153	0	VAL A 1		3.074	3.248	24.840		26.32	0
MOTA	1154	CB	VAL A 1		2.895	1.850	27.883		26.94	C
MOTA	1155		l VAL A 1		4.136	1.310	27.193		27.73	C
MOTA	1156		2 VAL A 1		3.223	2.308	29.298		26.73	. C
MOTA	1157	N	MET A 1		1.363	1.852	25.145		26.48	И
MOTA	1158	CA			1.270	1.518	23.721		26.52	C
ATOM	1159				0.985	2.771	22.880		25.02	C
MOTA	1160		MET A 1		1.600	2.986	21.845		24.31	0
MOTA	1161				0.183	0.476	23.485		27.05	C
MOTA	1162				0.540	-0.900	24.001		30.45	C
MOTA	1163				1.843	-1.730	23.058		34.87	S
MOTA	1164				0.957	-2.028	21.496		36.94	C
MOTA	1165		ASP A 1		0.047	3.589	23.342		23.96	N
ATOM	1166				9.699	4.831	22.665		23.14	C
MOTA	1167		ASP A 1		0.890	5.781	22.550		21.93	C
ATOM	1168		ASP A 1		1.167	6.323	21.480		21.41	C
MOTA	1169				8.549	5.528	23.402		23.13	C
MOTA	1170	CG	ASP A 1	.01 1	7.250	4.762	23.293	1.00	24.08	

ATOM	1171	OD1	ASP	A	161	17.182	3.812	22.478	1.00	21.27		0
MOTA	1172	OD2	ASP			16.248	5.035	23.980	1.00			0
MOTA	1173	N	PHE	A	162	21.575	5.973	23.671	1.00	20.59		N
MOTA	1174	CA	PHE			22.712	6.859	23.765	1.00	19.97		С
MOTA	1175	С	PHE			23.802	6.409	22.809	1.00	19.19		С
ATOM	1176	0	PHE	Α.	162	24.410	7.213	22.160	1.00	18.98		0
MOTA	1177	CB	PHE			23.223	6.859	25.220	1.00	20.44		С
ATOM	1178	CG	PHE			24.386	7.755	25.470	1.00	20.78		С
A TOM	1179		PHE			24.206	9.107	25.673	1.00	25.50		С
ATOM	1180		PHE			25.662	7.245	25.542	1.00			С
ATOM	1181		PHE			25.290	9.930	25.935	1.00			С
ATOM	1182		PHE			26.755	8.072	25.795	1.00			С
ATOM	1183	CZ	PHE			26.572	9.394	26.001	1.00			С
ATOM	1184	N	LEU			24.062	5.115	22.744	1.00			N
ATOM	1185	CA	LEU			25.084	4.597	21.838		19.42		С
ATOM	1186	C	LEU			24.715	4.804	20.361		18.63	-	C
ATOM ATOM	1187 1188	O	LEU			25.585	4.831	19.493	1.00			0
ATOM	1189	CB CG	LEU			25.297	3.115	22.104	1.00			C
ATOM	1190		LEU LEU			25.988 25.980	2.812 1.319	23.422 23.651		20.88		C
ATOM	1191		LEU			27.407	3.368	23.396		21.73		C
ATOM	1192	N N	GLY			23.419	4.917	20.104		18.01		N
ATOM	1193	CA	GLY			22.889	5.158	18.779		18.55		C
ATOM	1194	C	GLY			22.873	6.622	18.355		18.40		c
ATOM	1195	Ö	GLY			22.406	6.921	17.256		19.24		ŏ
ATOM	1196	N	PHE			23.365	7.521	19.209		17.50		N
MOTA	1197	CA	PHE			23.493	8.913	18.831		17.67		C
ATOM	1198	С	PHE	Α	165	24.497	8.955	17.663		17.49		С
MOTA	1199	0	PHE	Α	165	25.293	8.028	17.497	1.00	16.10		0
MOTA	1.200	CB	PHE			23.984	9.753	20.018	1.00	17.47		C
MOTA	1201	CG			165	22.932	10.004	21.098	1.00	18.51		С
ATOM.	1202		PHE			21.645	9.479	21.009	1.00	19.26		С
MOTA	1203		PHE			23.242	10.784	22.203		18.52		С
ATOM	1204		PHE			20.697	9.730	21.996		18.44		С
ATOM	1205		PHE			22.303	11.030	23.199		18.52		C
ATOM	1206	CZ			165	21.032	10.500	23.100		18.90		C
ATOM ATOM	1207 1208	N CA			166 166	24.466	10.009	16.854 15.712		17.77		N
ATOM	1209	C			166	25.393 26.787	10.110 10.622	16.129		18.29 18.73		C
ATOM	1210	Ö			166.	27.156	11.795	15.897		19.54	•	Ö
ATOM	1211	СВ			166	24.793	10.972	14.598		17.92		C
ATOM	1212	CG			166	25.571	10.861			17.28		c
ATOM	1213		ASN			26.679	10.289	13.262		16.53		ŏ
ATOM	1214		ASN			24.994	11.395	12.204		12.92		N
ATOM	1215	N			167	27.527	9.739	16.789		19.26		N
MOTA	1216	CA			167	28.867	10.035	17.264		19.76		С
MOTA	1217	С			167	29.785	10.266	16.084	1.00	19.88		С
ATOM	1218	0			167	30.731	11.031	16.169	1.00	19.35		0
ATOM	1219	CB			167	29.384	8.864	18.130		19.92		С
ATOM	1220	CG			167	28.556	8.728	19.351		20.39		С
ATOM	1221	CD1			167	27.686	7.727	19.656		20.85		С
MOTA	1222		TRP			28.445	9.686	20.400		20.99		С
MOTA	1223		TRP			27.059	7.995	20.851		21.18		N
ATOM	1224	CE2			167	27.509	9.194	21.325		20.70		C
MOTA	1225		TRP			29.065	10.916	20.664		21.55		C
ATOM ATOM	1226 1227		TRP TRP			27.183	9.871	22.488		22.63		C
ATOM	1227	CH2			167	28.731 27.789	11.589 11.071	21.804 22.706		21.78 22.79		C
ATOM	1229	N			168	27.769	9.577	14.979		20.07		N
ATOM	1230	CA			168	30.374	9.759	13.818		20.50		C
ATOM	1231	C			168	30.396	11.237	13.421		20.67		C
												•

ATOM	1232 0	ASN	A 168	31.465			1.00 19.54
ATOM	1233 CF	B ASN	A 168	29.917			1.00 20.87
ATOM	1234 CC	3 ASN	A 168	30.818			1.00 22.96
ATOM			A 168	32.027	8.923	11.522	1.00 25.54
ATOM			A 168	30.247	9.578	10.295	1.00 23.09
	1237 N		A. 169	29.211	11.844	13.338	1.00 20.57
ATOM	1238 C		A 169	29.106	13.226	12.917	1.00 20.23
ATOM			A 169	29.653	14.188	13.972	1.00 20.59
ATOM			A 169	30.367	15.118	13.634	1.00 20.09
MOTA	1240 0			27.662	13.618	12.570	1.00 20.35
MOTA	1241 C		A 169		15.101	12.238	1.00 19.49
ATOM	1242 C		A 169	27.542		11.026	1.00 19.03
MOTA			A 169	27.769	15.693	13.137	1.00 20.25
MOTA			A 169	27.203	16.157		1.00 20.25
MOTA			P A 169	27.578	17.052	11.117	
MOTA	1246 C		P A 169	27.244	17.366	12.406	
ATOM	1247 C		PA 169	26.874	16.207	14.492	1.00 20.60
MOTA	1248 C		PA 169	26.964	18.600	12.975	1.00 21.03
MOTA	1249 C	Z3 TRE	P A 169	26.614	17.433	15.064	1.00 23.09
MOTA		H2 TRI	P A 169	26.649	18.621	14.297	1.00 23.61
MOTA	1251 N	1 ILI	E A 170	29.326	13.979	15.239	1.00 20.47
ATOM		CA ILI	E A 170	29.759	14.926	16.241	1.00 20.67
ATOM ·			E A 170	31.262	14.772	16.567	1.00 21.18
ATOM			E A 170	31.943	15.758	16.836	1.00 21.20
ATOM			E A 170	28.842	14.892	17.483	1.00 20.61
ATOM			E A 170	28.900	16.231	18.221	1.00 20.05
			E A 170	29.191	13.755	18.402	1.00 19.89
MOTA			E A 170	27.865	16.353	19.329	1.00 21.00
MOTA			N A 17.1	31.780	13.556	16.527	1.00 20.74
MOTA			N A 171	33.214	13.355	16.715	1.00 21.80
MOTA				34.024	14.093	15.634	1.00 22.34
MOTA			N A 171	35.093	14.652	15.916	1.00 21.98
MOTA			N A 171	33.581	11.857	16.718	1.00 21.55
MOTA			SN A 171		11.124	17.981	1.00 21.20
MOTA			SN A 171	33.111	11.724	18.963	1.00 21.35
MOTA			SN A 171	32.637		17.962	1.00 21.35
MOTA			SN A 171	33.263		14.400	1.00 13.30
MOTA			rs A 172	33.529			1.00 24.09
MOTA	1268		(S A 172	34.218		13.353	1.00 24.03
MOTA	1269 [.]		YS A 172	34.167		13.656	
MOTA	1270		YS A 172	35.166		13.511	1.00 23.54
MOTA	1271		YS A 172	33.669		11.961	1.00 24.58
· ATOM	1272	CG L	YS A 172	34.087			1.00 27.56
MOTA	1273 `	CD L	YS A 172	33.653			
MOTA	1274	CE L	YS A 172	34.323			
MOTA	1275	NZ L	YS A 172	34.357			
MOTA	1276	N G	LN A 173	33.019			
ATOM	1277	CA G	LN A 173	32.914			
MOTA	1278	C G	LN A 173	33.960	18.578		
MOTA	1279		LN A 173	34.739	19.500	15.374	
MOTA	1280		LN A 173	31.517	7 18.590		
ATOM	1281		LN A 173	30.453	18.619	13.916	
ATOM	1282		LN A 173	30.75		12.851	1.00 25.08
MOTA	1283		LN A 173	31.19		13.157	1.00 26.69
	1284		LN A 173	30.51			. 1.00 23.36
MOTA			LN A 174	33.96			
MOTA			LN A 174	34.92			
MOTA			LN A 174	36.36			
ATOM			SLN A 174	37.13			
ATOM				34.78			
MOTA			SLN A 174 SLN A 174	35.68			
MOTA				35.59			
MOTA			JLN A 174	35.22			
MOTA	1292	OE1	GLN A 174	33.22	2 14.00		

ATOM	1293	NE2	GLN	Α	174	35.90	1 1	15.803	22.084	1.00	23.63 [.]		N
ATOM	1294	N	GLY			36.70		7.080	16.334	1.00			
			GLY										N
MOTA	1295	CA			-	38.00		L7.028	15.696	1.00			С
ATOM	1296	С	GLY			38.26		L8.209	14.768	1.00	25.21		C
MOTA	1297	0	GLY	A	175	39.31	0 1	18.842	14.854	1.00	25.60		0
MOTA	1298	N	LYS	Α.	176	37.32	7 1	L8.518	13.888		25.81		N
MOTA	1299	CA	LYS			37.49		19.634	12.961	1.00			
													C
ATOM	1300	C	LYS			37.71		20.997	13.638		26.95		С
MOTA	1301	0	LYS			38.49		21.803	13.136		26.74		0
MOTA	1302	CB	LYS	Α	176	36.25	6	19.778	12.077	1.00	27.35		C
ATOM	1303	CG	LYS	Α	176	36.09	3 :	18.716	11.009	1.00	29.87	•	С
MOTA	1304	CD	LYS	Α	176	34.89		19.085	10.137		33.21		Č
ATOM	1305	CE	LYS			33.94		17.932	9.961		35.30		c
ATOM	1306	NZ	LYS			32.55		18.388	9.643		37.22		N
MOTA	1307	N	ARG	A	177	37.03		21.257	14.749	1.00	26.93		. N
ATOM	1308	CA	ARG	Α	177	37.15	3 2	22.539	15.435	1.00	27.36		С
ATOM	1309	С	ARG	Α	177	38.24	1 :	22.611	16.509	1.00	26.63		С
ATOM	1310	0	ARG			38.40		23.650	17.135		25.85		Ö
ATOM	1311	СВ	ARG			35.83		22.902					
									16.114		27.86		C
MOTA	1312	CG	ARG			34.62		22.712	15.267		29.88		С
ATOM.	1313	CD	ARG			34.65	33	23.460	13.973	1.00	32.39		С
MOTA	1314	NE	ARG	Α	177	33.68	33 :	22.854	13.084	1.00	34.54		N
ATOM	1315	CZ	ARG	Α	177	33.84	1 :	22.701	11.790	1.00	37.31		С
ATOM	1316	NH1			177 .	34.95		23.110	11.189		38.34		N
ATOM	1317		ARG			32.87		22.126	11.088		38.88		N
MOTA	1318	N	GLY			38.95		21.510	16.743	-	26.35		N
MOTA	1319	CA	GLY			39.99		21.470	17.753	1.00	25.46		С
ATOM	1320	С	GLY	Α	178	39.47	73	21.514	19.176	1.00	25.27		С
MOTA	1321	0	GLY	Α	178	40.21	.3	21.818	20.123	1.00	25.46		0
MOTA	1322	N	TRP			38.19		21.202	19.359		24.30		N
ATOM	1323	CA			179	37.63		21.260	20.692		24.02		Ċ
ATOM	1324	C			179								
						38.29		20.266	21.638		23.85		C
MOTA	1325	0			179	38.95		19.333	21.226		22.62		0
MOTA	1326	CB	TRP			36.13		21.011	20.674	1.00	23.73		С
MOTA	1327	CG			179	35.34	16	22.061	19.962	1.00	23.92		С
MOTA	1328	CD1	TRP	A	179 ·	35.78	37	23, 291	19.531	1.00	22.69		С
ATOM	1329	CD2	TRP	Α	179	33.96		21.981	19.594		23.74		С
ATOM	1330		TRP			34.76		23.968	18.912		24.45		N
ATOM	1331		TRP			33.63		23.183 _.					C
ATOM	1332										24.47		
			TRP			32.98		21.002	19.730		23.10		C.
ATOM	1333		TRP			32.37		23.422	18.414		23.69		C.
MOTA	1334				179	31.73	33	21.241		1.00	21.89		С
ATOM	1335	CH2	TRP	Α	179	31.43	35	22.445	18.573	1.00	23.90		С
ATOM	1336	. N	GLY	Α	180	38.08		20.499	22.925		24.08		N
ATOM	1337	CA			180			19.558	23.941		24.08		C
ATOM	1338	C			180	37.43		18.476	24.103				c
	1339										24.64		
ATOM		0			180	36.61		18.234	23.202		24.66		0
ATOM	1340	N			181	37.43	37	17.830	25.261	1.00	24.77		N
MOTA	1341	CA	GLN	Α	181	36.57		16.682	25.471	1.00	25.23		C
ATOM	1342	С	GLN	Α	181	35.11	17	17.039	25.725	1.00	24.50		С
ATOM	1343	0			181	34.77		18.151	26.149		24.42		0
ATOM	1344	СВ			181	37.09		15.847	26.646		25.76		č
ATOM	1345	CG											
					181	36.72		16.409	28.025		28.85		C
ATOM	1346	CD			181	37.04		15.434	29.156		33.38		С
ATOM	1347		GLN			38.18		15.003	29.293		36.10		0
ATOM	1348	NE2	GLN	A	181	36.04	44	15.085	29.958	1.00	36.04	•	N
ATOM	1349	N	LEU	A	182	34.26	62	16.078	25.423		23.71		N
ATOM	1350	CA			182	32.85		16.110	25.792		23.70		Ċ
ATOM	1351	C			182	32.87		16.040	27.317		22.68		c
ATOM	1352	0			182								
						33.40		15.079	27.849		21.72		0
MOTA	1353	CB	ııεU	A	182	32.17	19	14.836	25.273	1.00	23.82		С

ATOM	1354	CG :	LEU A	. 1	.82	30.661	14.693	25.199	1.00	26.38	С	
MOTA	1355	CD1	LEU P	1	L82	30.243	13.231	25.368		26.04	С	
MOTA	1356		LEU F			29.977	15.501	26.192		29.73	С	
MOTA	1357		THR A			32.323	17.031	28.021		21.93	N	
MOTA	1358		THR A			32.300	16.971	29.484		21.44	c	
MOTA	1359		THR F			31.004	16.388	29.984		21.27	C	
MOTA	1360		THR A			30.972	15.766	31.032		21.29	0	
ATOM	1361		THR A			32.490	18.362	30.150		21.73	0	
ATOM	1362		THR A			31.463	19.257 19.015	29.715 29.725		20.35	C	
ATOM	1363		THR A			33.796 29.918	16.590	29.725		21.42	Ŋ	
ATOM	1364 1365		SER A			28.649	16.053	29.689		21.45	C	
ATOM ATOM	1366		SER A			27.537	16.272	28.714		21.46	c	
ATOM	1367	Ö	SER A			27.672	17.031	27.753		21.17	ō	
MOTA	.1368	СВ	SER A			28.243	16.687	31.006		21.74	C	
ATOM	1369	OG	SER A			27.919	18.049	30.845		23.24	0	
ATOM	1370	N	ASN 2			26.445	15.575	28.982		21.21	N	
MOTA	1371	CA	ASN 2			25.216	15.712	28.245	1.00	22.29	С	
ATOM	1372	С	ASN :			24.154	16.005	29.273	1.00	22.08	С	
MOTA	1373	0	ASN .			23.886	15.184	30.135	1.00	22.25	0	
ATOM	1374	CB	ASN .	A	185	24.856	14.416	27.497	1.00	22.67	С	
ATOM	1375	CG	ASN .	Α	185	25.885	14.037	26.454		23.57	C	
MOTA	1376		ASN .			26.646	13.097	26.655		27.51	0	
MOTA	1377		ASN			25.905	14.754	25.329		24.27	N	
MOTA	1378	N	LEU			23.574	17.189	29.202		22.01	Ŋ	
MOTA	1379	CA	LEU			22.529	17.563	30.135		22.03	C	
MOTA	1380	C	LEU			21.170	17.219	29.558		22.00	·	
MOTA	1381	0	LEU			20.844	17.592	28.435		22.34	· c	
MOTA	1382	CB	LEU			22.578	19.065	30.423 31.588		21.68 22.25		
MOTA	1383	CG CD1	LEU LEU			21.707 22.252	19.538 18.985	32.891		22.43		
ATOM ATOM	1384 1385		LEU			21.643	21.098	31.648		23.35	Č	
ATOM	1386	N N	LEU			20.377	. 16.518	30.344		22.19	1	
MOTA	1387	CA	LEU			19.009	16.198	29.979		21.95	Ċ	
ATOM	1388	C	LEU			18.149	17.286	30.603		21.91		
ATOM	1389	ō	LEU			18.232	17.521	31.823		21.61		2
ATOM	1390	CB	LEU			18.616	14.830	30.527	1.00	21.55		C
MOTA	1391	CG	LEU			17.129	14.488	30.477		22.78		C
MOTA	1392	CD1	LEU	A	187 .	16.616	14.429	29.054	1.00	23.66		С
MOTA	1393	CD2	LEU	Α	·187	16.866	13.143	31.174		22.84		С
MOTA	1394	И	LEU	A	188	17.348	17.956	29.770		21.56		N
MOTA	1395	CA	LEU			16.461	19.000	30.227		22.26		C
MOTA	1396	С	LEU			14.993	18.662			22.55		C
MOTA	1397	0	LEU			14.588	18.517			23.16		0
ATOM	1398	CB			188	16.827	20.327			22.84		C C
ATOM	1399	CG			188	18.244	20.840			22.60		C
ATOM	1400		LEU			18.967 18.177	21.111 22.088			24.56		C
MOTA MOTA	1401 1402	N	LEU		188. 189	14.181	18.577			22.15		N
ATOM	1402				189	12.769				22.34		C
ATOM	1404	C			189	11.996				22.37		Č
ATOM	1405	Ö			189	12.072				22.77		0
ATOM	1406				189	12.377				21.60		С
ATOM	1407		. ILE			13.254				21.85		С
ATOM	1408		ILE			10.928				22.51		С
ATOM	1409		ILE			. 12.918				23.06		С
MOTA	1410				190	11.276	20.186			22.37		N
MOTA	1411	CA	GLY	A	190	10.587				22.29		С
MOTA	1412				190	9.124				0 22.48		С
MOTA	1413				190	8.652				0 22.39		0
MOTA	1414	N	MET	A	191	8.402	22.134	31.687	1.0	0 22.74		N

ATOM	1415	CA	MET	Α	191		6.991	22.339	31.467	1.00	23.16	С	
ATOM	1416	С	MET	Α	191		6.838	23.482	30.478		22.94	С	
MOTA	1417	0	MET	A	191		7.738	24.329	30.338		23.03	0	
ATOM	1418	CB	MET	Α	191		6.283	22.673	32.784		23.69	C	
MOTA	1419	CG	MET	Α	191		6.224	21.513	33.741		25.02	C	
MOTA	1420	SD	MET	A.	191		5.664	21.927	35.415		28.11	s	
MOTA	1421	CE	MET	Α	191		4.016	22.460	35.097		28.35	C	
ATOM	1422	N	GLU	A	192		5.712	23.492	29.773		22.60	N	
MOTA	1423	CA	GLU	A	192		5.410	24.544	28.810		22.83	C	
ATOM	1424	С	GLU	Α	192		5.495	25.895	29.490		22.51	C	
ATOM	1425	0	GLU	Α	192		5.062	26.046	30.614		22.41	ō	
ATOM	1426	CB	GLU	Α	192		4.005	24.342	28.249		22.86	Č	
ATOM	1427	CG	GLU				2.925	24.367	29.315		24.36	c	
MOTA	1428	CD	GLU	Α	192		1.572	23.891	28.814		25.71	C	
ATOM	1429	OE1	GLU	Α	192		1.503	23.294	27.718		25.51	Ö	
MOTA	1430	OE2	GLU	A	192		0.582	24.128	29.525		26.30	ō	
ATOM	1431	N	GLY	A	193		6.069	26.888	28.828		22.95	N	
MOTA	1432	CA	GLY	A	193		6.185	28.199	29.444		22.50	C	
MOTA	1433	С	GLY	Α	193		7.465	28.414	30.254		22.36	Č	
MOTA	1434	0	GLY	A	193	. •	7.756	29.544	30.602		23.08	ō	
MOTA	1435	N	ASN	Α	194		8.219	27.361	30.566		21.60	N	
MOTA	1436	CA	ASN	Α	194		9.456	27.506	31.341		21.44	C	
MOTA	1437	С	ASN	A	194		10.489	28.320	30.581		21.19	Č	
ATOM	1438	0	ASN	Α	194		10.635	28.134	29.372		22.08	Ö	
ATOM	1439	CB	ASN	Α	194		10.099	26.147	31.629		21.05	Č	
MOTA	1440	CG	ASN	Α	194		9.494	25.435	32.801		20.86	č	
MOTA	1441	OD1	ASN	Α	194		8.509	25.883	33.385		22.48	ō	
ATOM	1442	ND2	ASN	A	194		10.092	24.312	33.167		17.74	N	
ATOM	1443	N	VAL	Α	195		11.213	29.183	31.290		20.69	N	
ATOM	1444	CA	VAL	Α	195		12.268	29.993	30.701		20.84	C	
MOTA	1445	С	VAL	Α	195		13.572	29.854	31.450		20.06	c	
ATOM	1446	0	VAL	Α	195		13.601	29.874	32.681		20.75	ő	
MOTA	1447	CB	VAL	Α	195		11.903	31.502	30.686		21.41	c	
ATOM	1448	CG1	VAL	Α	195		13.081	32.357	30.219		22.24	c	
MOTA	1449	CG2	VAL	Α	195		10.666	31.767	29.843		22.30	c	
MOTA	1450	N	THR	A	196		14.651	29.673	30.702		19.51	N	
MOTA	1451	CA	THR	A	196		15.993	29.737	31.257		19.52	C	
MOTA	1452	С	THR	A	196		16.487	31.117	30.820		19.98	c	
MOTA	1453	0	THR	Α	196		16.653	31.352	29.620		19.56	ō	
ATOM	1454	CB	THR	Α	196		16.896	28.677	30.675		19.26	C	
ATOM	1455	OG1					16.526	27.366	31.162		21.13	Ō	
MOTA	1456	CG2	THR				18.309	28.886	31.185		19.85	C	:
MOTA	1457	N	PRO				16.627	32.043	31.767		20.27	. N	
MOTA	1458	CA			197		17.046	33.412	31.463	1.00	20.52	С	
MOTA	1459	С			197		18.431	33.497	30.836	1.00	20.89	С	
MOTA	1460	0	PRO				19.277	32.609	31.025	1.00	20.66	0	
MOTA	1461	CB	PRO	Α	197		17.018	34.099	32.825	1.00	21.22	С	
MOTA	1462	CG	PRO				16.144	33.263	33.657	1.00	21.01	С	
MOTA	1463	CD	PRO				16.309	31.872	33.189	1.00	20.28	С	
MOTA	1464	N	ALA				18.633	34.577	30.089		20.28	N	
MOTA	1465	CA	ALA	Α	198		19.841	34.817	29.341		20.22	C	
MOTA	1466	С	ALA	Α	198		21.130	34.634	30.146	1.00	20.58	C	
MOTA	1467	0	ALA				21.284	35.186	31.235	1.00	19.91	Ó	
MOTA	1468	СВ	ALA				19.791	36.222	28.759	1.00	20.52	Ċ	
ATOM	1469	N			199		22.062	33.891	29.563		20.87	N	
ATOM	1470	CA	HIS				23.371	33.646	30.158		21.41	Ċ	
ATOM	1471	С	HIS				24.281	33.168	29.063		21.82	c	
MOTA	1472	0	HIS				23.826	32.892	27.943		21.80	ō	
ATOM	1473	CB	HIS				23.305	32.534	31.198		21.44	Ċ	
ATOM	1474	CG	HIS				22.915	31.220	30.617		22.21	c	
MOTA	1475	ND1	HIS	Α	199		21.619	30.940	30.253		21.93	N	
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			00 644	20 120	30.296	1.00 22.04
MOTA	1476	CD2 HIS A 199	23.644	30.120		
MOTA	1477	CE1 HIS A 199	21.561	29.721		1.00 23.76
ATOM	1478	NE2 HIS A 199	22.777	29.214		1.00 22.57
MOTA	1479	N TYR A 200	25.568	33.060		1.00 22.40
MOTA	1480	CA TYR A 200	26.536	32.456		1.00 22.34
MOTA	1481	C TYR A. 200	27.225	31.316	29.197	1.00 22.03
ATOM	1482	O TYR A 200	27.328	31.330	30.425	1.00 21.90
MOTA	1483	CB TYR A 200	27.544	33.458	27.924	1.00 22.22
	1484	CG TYR A 200	28.517	34.051	28.924	1.00 22.16
ATOM		CD1 TYR A 200	29.746	33.454	29.171	1.00 21.36
MOTA	1485		28.236	35.246	29.565	1.00 22.58
MOTA	1486	CD2 TYR A 200		33.240	30.052	1.00 21.48
MOTA	1487	CE1 TYR A 200	30.638	35.806	30.462	1.00 21.46
MOTA	1488	CE2 TYR A 200	29.128			1.00 21.40
MOTA	1489	CZ TYR A 200	30.334		30.695	1.00 22.03
MOTA	1490	OH TYR A 200	31.230	35.733	31.593	
ATOM	1491	N ASP A 201	27.681	30.310	28.444	1.00 22.42
MOTA	1492	CA ASP A 201	28.381	29.152	29.048	1.00 22.10
MOTA	1493	C ASP A 201	29.801	29.142	28.531	1.00 21.96
ATOM	1494	O ASP A 201	30.018	29.601	27.433	1.00 22.26
ATOM	1495	CB ASP A 201	27.722	27.840	28.661	1.00 21.97
ATOM	149.6	CG ASP A 201	26.311	27.714	29.181	1.00 21.99
ATOM	1497	OD1 ASP A 201	26.126	27.649	30.421	1.00 22.61
	1498	OD2 ASP A 201	25.330	27.624	28.412	1.00 19.35
MOTA			30.769	28.620	29.283	1.00 21.66
MOTA	1499		32.146	28.612	28.773	1.00 23.16
MOTA	1500	CA GLU A 202		27.334	28.035	1.00 23.38
MOTA	1501	C GLU A 202	32.515	26.951	28.049	1.00 25.48
MOTA	1502		33.684			1.00 23.46
MOTA	1503		33.178	28.774	29.897	
MOTA	1504		33.110	30.064	30.681	1.00 26.52
MOTA	1505	CD GLU A 202	34.233	30.132	31.704	1.00 28.11
MOTA	1506	OE1 GLU A 202	34.207		32.698	1.00 29.06
MOTA	1507	OE2 GLU A 202	35.148		31.490	1.00 31.04
MOTA	1508		31.538	26.632	27.476	1.00 22.70
ATOM	1509		31.808	25.451	26.685	1.00 22.01
ATOM	1510		31.049		25.373	1.00 21.93
ATOM	1511		30.113			1.00 22.49
ATOM	1512		31.409			1.00 22.02
ATOM	1513		32.287			1.00 22.33
	1514		32.103			1.00 23.14
ATOM			31.948			1.00 21.46
ATOM	1515		32.138			1.00 21.21
MOTA	1516		31.486			
ATOM		N GLN A 204				1.00 21.45
MOTA	1518		30.806			1.00 21.12
MOTA	1519		29.610			1.00 21.12
ATOM	1520		29.673			_
MOTA	152		31.740			
MOTA	152		33.033			
MOTA	152	3 CD GLN A 204	32.856			
MOTA		4 OE1 GLN A 204	31.741			
ATOM			33.966	5 26.776	20.594	
ATOM			28.522		22.580	
ATOM			27.29			1.00 21.04
ATOM			26.529			1.00 21.25
ATOM			26.160			
	_		26.38			
ATOM			25.11			
ATOM			24.75		_	
MOTA						
ATOM	_		24.40			
ATOM			26.31			
MOTA			25.33			
ATOM	153	6 C PHE A 206	24.08	5 20.86	9 21.150	7 1.00 13.43

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ATOM	1537	0	PHE	A	206	2	24.094	19.939	21.959	1.00	19.15		0
MOTA	1538	CB	PHE	Α	206	2	25.849	20.049	19.545		20.09		Ċ
ATOM	1539	CG	PHE	A	206		26.786	20.442	18.454		19.77		Č
MOTA	1540	CD1	PHE	A	206	2	26.371	21.294	17.453	1.00	22.21		Ċ
ATOM	1541	CD2	PHE	Α	206		28.079	19.973	18.435		20.21		Ċ
ATOM	1542	CE1	PHE	A·	206	2	27.213	21.643	16.434		22.06		c
MOTA	1543		PHE				28.941	20.336	17.418		20.66		c
ATOM	1544	CZ	PHE				28.504	21.190	16.427		22.18		c
MOTA	1545	N	PHE				23.009	21.596	20.869		18.42	•	N
ATOM	1546	CA	PHE				21.760	21.590	21.620		18.78	•	c
MOTA	1547	С	PHE				20.732	20.841	20.804		19.36		c
MOTA	1548	0	PHE				20.241	21.359	19.818		19.26		ŏ
MOTA	1549	СВ	PHE				21.366	23.063	21.836		18.70		c
ATOM	1550	CG	PHE				20.120	23.301	22.635		17.94		č
MOTA	1551		PHE				18.899	23.404	22.007		17.78		c
MOTA	1552		PHE				20.188	23.548	23.989		18.50		c
ATOM	1553		PHE				17.772	23.684	22.713		19.52	•	c
MOTA	1554		PHE				19.052	23.823	24.705		20.66		č
MOTA	1555	CZ	PHE				17.836	23.909	24.053		19.44		c
MOTA	1556	N	ALA				20.435	19.618	21.234		19.90		N
ATOM	1557	CA	ALA				19.628	18.670	20.469		20.17		c
ATOM	1558	С	ALA					. 18.541	20.991		20.52		Č
ATOM	1559	Ō	ALA				17.971	17.946	22.047		20.61		ŏ
MOTA	1560	СВ	ALA				20.294	17.308	20.494		19.33		Ċ
ATOM	1561	N			209		17.270	19.076	20.219		20.94		N
MOTA	1562	CA			209		15.880	19.062	20.627		20.82		C
ATOM	1563	С			209		15.227	17.712	20.323		20.75		Č
MOTA	1564	Ō			209		15.401	17.129	19.224		19.59		ŏ
MOTA	1565	CB			209		15.141	20.216	19.961		20.91		č
MOTA	1566	CG			209		13.735	20.431	20.463		20.52		č
ATOM	1567	CD			209		13.673	20.840	21.928		20.69		č
ATOM	1568	OE1			209		14.702	21.155	22.562		19.72		ŏ
MOTA	1569		GLN				12.460	20.852	22.473		19.21		N
MOTA	1570	N			210		14.442	17.248	21.296		20.72		N
ATOM	1571	CA			210		13.853	15.922	21.252		21.43		C
ATOM	1572	С			210		12.334	15.911	21.292		21.72		č
MOTA	1573	0			210		11.728	15.195	20.534		22.12		Ö
MOTA	1574	CB			210		14.396	15.095	22.424		21.84		Č
ATOM	1575	CG1			210		15.859	14.733	22.156		22.48		č
MOTA	1576	CG2	ILE				13.581	13.832	22.622		21.83		Ċ
MOTA	1577		ILE				16.631		23.382		24.34		Č
MOTA	1578	N	LYS	Α	211		11.728	16.677	22.188		22.08		N
MOTA	1579	CA			211		10.279	16.715	22.319		21.72		Ċ
ATOM	1580	С			211		9.858	18.130	22.564		21.67		Ċ
ATOM	1581	0			211		10.468	18.841	23.372		20.87		ō
ATOM	1582	CB			211		9.797	15.856	23.487		22.44		Ċ
ATOM	1583	CG	LYS	Α	211 -		8.267	15.562	23.479		23.29	•	Ċ
MOTA	1584	CD			211 ·		7.791	15.022	24.824		25.02		Ċ
MOTA	1585	CE	LYS	A	211		6.494	14.215	24.757		26.00		Ċ
ATOM	1586	NZ	LYS	A	211		5.561	14.522	23.634		26.43		N
MOTA	1587	N	GLY	Α	212		8.798	18.541	21.875		21.35		N
ATOM	1588	CA			212		8.306	19.891	21.994		21.71		C
ATOM	1589	С	GLY	Α	212		9.195	20.906	21.297		21.63		C
ATOM	1590	0			212		10.150	20.572	20.591		21.32		ŏ
MOTA	1591	N			213		8.871	22.166	21.522		22.35		N
ATOM	1592	CA			213		9.533	23.279	20.862		22.42		C
MOTA	1593	С			213		10.028	24.293	21.868		22.33		c
MOTA	1594	0			213		9.340	24.589	22.853		21.55		Ö
ATOM	1595	CB			213		8.556	23.951	19.916		23.46		Č
ATOM	1596	CG	TYR	A	213		8.114	23.034	18.815		24.81		Č
MOTA	1597	CD1	TYR				7.100	22.112	19.020		28.16		Ċ
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ATOM	1598	CD2	TYR A	213	8.751	23.051	17.589	1.00 26.74	С
MOTA	1599	CE1	TYR A	213	6.716	21.237	18.011	1.00 28.91	C
MOTA	1600		TYR A		8.378	22.193	16.585	1.00 28.63	C
MOTA	1601		TYR A		7.366	21.295	16.795	1.00 29.44	С
MOTA	1602		TYR A		7.013	20.456	15.756	1.00 33.67	0
ATOM	1603		LYS A		11.239	24.788	21.609	1.00 21.60	N
MOTA	1604		LYS A		11.875	25.793	22.414	1.00 21.89	C
MOTA	1605		LYS A		12.312	26.947	21.528	1.00 21.62	C O
MOTA	1606		LYS A		12.878	26.747 25.239	20.442 23.140	1.00 22.07 1.00 22.10	C
ATOM ATOM	1607 1608	CB CG	LYS A		13.103 12.796	24.385	24.338	1.00 22.10	c
ATOM	1609	CD	LYS A		14.103	23.893	24.964	1.00 24.24	č
ATOM	1610	CE	LYS A		13.923	23.478	26.402	1.00 23.54	Ċ
ATOM	1611	NZ	LYS A		15.169	22.872	26.951	1.00 22.10	N
ATOM	1612	N	ARG A		12.007	28.156	21.974	1.00 20.97	N
ATOM	1613	CA	ARG A		12.447	29.347	21.277	1.00 20.73	С
ATOM	1614	С	ARG F		13.778	29.724	21.900	1.00 20.03	С
ATOM	1615	0	ARG A		13.885	29.828	23.113	1.00 19.70	0
MOTA	1616	CB	ARG A	A 215	11.461	30.470	21.493	1.00 21.30	С
MOTA	1617	CG	ARG A		11.754	31.760	20.726	1.00 22.21	C
MOTA	1618	CD	ARG A	1 215	11.177	32.925	21.473	1.00 24.71	С
MOTA	1619	NE	ARG A		11.122	34.156	20.715	1.00 25.47	N
MOTA	1620	CZ	ARG A		10.479	35.235	21.130	1.00 26.28	C
MOTA	1621		ARG A		9.844	35.245	22.299	1.00 26.07	N
MOTA	1622		ARG A		10.483	36.314	20.384	1.00 28.83	N
ATOM	1623	N		A 216	14.794	29.877	21.074	1.00 19.45	N
ATOM	1624	ÇA		A 216	16.116	30.219	21.554	1.00 19.58	C
MOTA	1625	C		A 216	16.503	31.587	20.993	1.00 19.92	0
MOTA	1626 1627	O CB		A 216 A 216	16.503 17.110	31.774 29.186	19.789 21.073	1.00 20.16 1.00 20.01	C
ATOM .	1628	SG		A 216	16.693	27.450	21.073	1.00 20.01	S
ATOM	1629	N		A 217	16.812	32.530	21.878	1.00 21.33	N
ATOM	1630	CA		A 217	17.286	33.845	21.504	1.00 19.58	C
ATOM		· C		A 217	18.742	33.961	21.937	1.00 19.21	C
ATOM	1632	Ö		A 217	19.055	33.849	23.126	1.00 19.05	0
ATOM	1633	CB		A 217	16.424	34.943	22.168	1.00 19.88	· C
MOTA	1634	CG1		A 217	14.926	34.687	21.878	1.00 20.56	С
MOTA	1635	CG2	ILE .	A 217	16.803	36.312	21.627	1.00 20.25	C
MOTA	1636	CD1	ILE .	A 217	13.984	35.692	22.488	1.00 20.99	С
MOTA	1637	N	LEU .	A 218	19.620		20.965	1.00 19.01	N
MOTA	1638	CA		A 218	21.048	34.271	21.222	1.00 19.61	C
ATOM	1639	С		À 218	21.568	35.682	20.970	1.00 20.43	c
ATOM	1640	0		A 218	21.018		20.136	1.00 19.76	0
ATOM	1641	CB		A 218	21.816		20.308	1.00 19.66	C
MOTA	1642	CG		A 218	21.906		20.778	1.00 19.74	C
ATOM ATOM	1643 1644			A 218 A 218	20.549 22.733		20.905 19.798	1.00 20.56 1.00 21.32	C
MOTA	1645	N N		A 219	22.626		21.700	1.00 21.32	N
ATOM	1646	CA		A 219	23.282		21.524	1.00 20.11	C
ATOM	1647	C		A 219	24.805		21.453	1.00 21.19	C
ATOM	1648	ō		A 219	25.351		22.257	1.00 21.20	ō
ATOM	1649	СВ		A 219	22.942		22.678	1.00 20.97	С
ATOM	1650	CG		A 219	21.463		22.954	1.00 20.44	С
ATOM	1651			A 219	20.821		23.846	1.00 21.46	C
MOTA	1652			A 219	20.724		22.334	1.00 22.49	С
MOTA	1653			A 219	19.472	37.790	24.108	1.00 22.33	C
MOTA	1654			A 219	19.387		22.605	1.00 21.32	С
ATOM	1655	CZ		A 219	18.760		23.480	1.00 21.50	C
ATOM	1656	N		A 220	25.485		20.498	1.00 21.20	N
MOTA	1657	CA		A 220			20.368	1.00 21.72	C
MOTA	1658	С	PRO	A 220	27.683	38.108	21.569	1.00 21.31	С

MOTA	1659	0			220	27.165	38.972	22.280	1.00 20.9	90	0
MOTA	1660	CB	PRO	A	220	27.302	38.341	19.120	1.00 21.4		c
MOTA	1661	CG			220	26.020	38.781	18.510	1.00 23.3		c
ATOM	1662	CD	PRO	A	220	24.938	38.637	19.508	1.00 22.2		Č
ATOM	1663	N			221	28.884	37.594	21.806	1.00 21.4		N
ATOM	1664	CA	PRO	A.	221	29.721	38.053	22.918	1.00 21.3		C
MOTA	1665	С			221	29.961	39.556	22.940	1.00 21.0		c
ATOM	1666	0			221	30.220	40.096	24.009	1.00 20.		ō
ATOM	1667	CB	PRO	A	221	31.032	37.325	22.681	1.00 21.4		Č
ATOM	1668	CG .	PRO	A	221	30.656	36.134	21.939	1.00 22.4		Ċ
MOTA	1669	CD	PRO	Α	221	29.522	36.510	21.041	1.00 21.5		C
ATOM	1670	N			222	29.877	40.225	21.792	1.00 21.4		N
MOTA	1671	CA			222	30.128	41.669	21.749	1.00 21.8		С
ATOM	1672	С			222	28.946	42.464	22.271	1.00 21.		С
MOTA	1673 ·				222	28.970	43.685	22.261	1.00 22.3	16	0
ATOM	1674	CB			222	30.568	42.148	20.355	1.00 21.8	85	С
ATOM	1675		ASP			29.433	42.151	19.325	1.00 24.8	83	С
ATOM	1676		ASP			28.311	41.668	19.585	1.00 25.3	32	0
ATOM	1677		ASP			29.595	42.607	18.186	1.00 29.3	30	0
MOTA	1678	N			223	27.916	41.775	22.748	1.00 21.9	94	N
ATOM	1679	CA			223		42.453	23.388	1.00 22.3	17	С
ATOM	1680	С			223	26.897	42.388	24.928	1.00 21.9		С
MOTA	1681	0			223	25.926	42.681	25.660	1.00 21.	70	0
ATOM.	1682	CB			223	25.456	41.911	22.832	1.00 22.8		С
MOTA	1683	CG			223	25.149	42.508	21.412	1.00 25.3		С
ATOM	1684	CD			223	23.728	42.283	20.965	1.00 27.8		С
ATOM	1685	OE1			223	22.801	42.473	21.750	1.00 30.0		0
MOTA	1686	NE2				23.543	41.850	19.709	1.00 29.		N
ATOM ATOM	1687	N			224	28.079	42.027	25.417	1.00 21.0		N
ATOM	1688	CA			224	28.363	42.035	26.860	1.00 21.		С
ATOM	1689 1690	C			224	27.886	43.350	27.527	1.00 21.		С
ATOM		O			224	27.240	43.315	28.561	1.00 21.3		0
ATOM	1691 1692	CB CG			224	29.883	41.874	27.076	1.00 20.		С
ATOM	1693		PHE		224	30.304	41.773	28.529	1.00 21.8		С
ATOM	1694	CD2			224	30.452	42.912	29.319	1.00 19.3		С
ATOM	1695	CE1				30.595	40.552	29.089	1.00 20.0		С
ATOM	1696		PHE			30.870	42.807	30.630	1.00 20.1		С
ATOM	1697	CZ			224	31.025 31.151	40.449	30.397	1.00 20.		C
ATOM	1698	N			225	28.195	41.579	31.171	1.00 20.9		С
ATOM	1699	CA			225	27.823	44.495	26.916	1.00 22.		N
ATOM	1700	C	GLU			26.337		27.466	1.00 23.0		C
ATOM	1701	Õ			225	25.928	46.042 46.946	27.574 28.311	1.00 22.		C
ATOM	1702	СВ			225	28.401	46.935	26.624	1.00 21.9		0
MOTA	1703	CG			225	29.886	47.133	26.857	1.00 24.7		C
ATOM	1704	CD			225	30.312	48.579	27.062	1.00 25.		C
ATOM	1705		GLU			29.745	49.317	27.942	1.00 39.		С
ATOM	1706		GLU			31.281	48.958	26.368	1.00 40.		0
MOTA	1707	N			226	25.539	45.258	26.836	1.00 40.		о И
ATOM	1708	CA			226	24.081	45.396	26.851	1.00 21.0		C
MOTA	1709	С			226	23.359	4.4.417	27.768	1.00 20.0		c
ATOM	1710	0			226	22.159	44.601	28.043	1.00 18.8		ō
ATOM	1711	CB			226	23.520	45.190	25.447	1.00 20.8		c
ATOM	1712	SG			226	24.194	46.296	24.190	1.00 22.3		s
ATOM	1713	N			227	24.085	43.399	28.256.	1.00 20.		N
MOTA	1714	CA			227	23.461	42.304	28.985	1.00 20.4		C
ATOM	1715	С	LEU			23.795	42.185	30.466	1.00 20.		C
MOTA	1716	0	LEU			23.180	41.398	31.187	1.00 20.		0
MOTA	1717	CB	LEU	A	227	23.737	41.003	28.232	1.00 21.2		c
ATOM	1718	CG	LEU	Α	227	22.865	40.993	26.963	1.00 22.9		c
MOTA	1719	CD1	LEU			23.373	40.023	25.929	1.00 24.9		c
											-

						70
ATOM	1720	CD2 LEU A 227	21.420			1.00 24.79
MOTA	1721	N TYR A 228	24.793			1.00 20.08
ATOM	1722	CA TYR A 228	25.060			1.00 19.66
ATOM	1723	C TYR A 228	25.061			1.00 19.95
ATOM	1724	O TYR A 228	24.229	41.697		1.00 19.69
ATOM	1725	CB TYR A 228	24.050	44.137	32.857	1.00 19.77
ATOM	1726	CG TYR A 228	24.028	45.481	32.119	1.00 19.37
ATOM	1727	CD1 TYR A 228	24.836	46.513	32.515	1.00 18.65
		CD2 TYR A 228	23.180	45.697		1.00 19.82
MOTA	1728	CE1 TYR A 228	24.819	47.759		1.00 20.56
ATOM	1729	CE2 TYR A 228	23.143	46.920		1:00 20.78
MOTA	1730		23.962	47.956	30.801	1.00 20.88
MOTA	1731		23.944	49.174	30.152	1.00 19.73
MOTA	1732	OH TYR A 228		40.981	32.941	1.00 19.99
MOTA	1733	N PRO A 229	26.028	39.781	33.768	1.00 20.44
MOTA	1734	CA PRO A 229	26.140		35.196	1.00 19.99
MOTA	1735	C PRO A 229	26.481	40.141		1.00 20.03
MOTA	1736	O PRO A 229	27.130	41.166	35.451	1.00 20.03
ATOM	1737	CB PRO A 229	27.334	39.043	33.157	
MOTA	1738	CG PRO A 229	28.125	40.130	32.541	1.00 21.04
ATOM	1739	CD PRO A 229	27.099	41.050	31.935	1.00 19.79
ATOM	1740	N TYR A 230	26.044	39.294	36.115	1.00 19.50
ATOM	1741	CA TYR A 230	26.348	39.458	37.511	1.00 19.17
ATOM	1742	C TYR A 230	27.860	39.464	37.704	1.00 19.14
MOTA	1743	O TYR A 230	28.598	39.060	36.832	1.00 18.83
ATOM	1744	CB TYR A 230	25.746	38.313	38.320	1.00 18.51
ATOM	1745	CG TYR A 230	24.253	38.411	38.531	1.00 18.95
ATOM	1746		23.368	37.949	37.560	1.00 18.39
ATOM.	1747		23.719	38.969	39.707	1.00 18.65
ATOM	1748		22.001	38.006	37.751	1.00 17.34
	1749		22.337	39.043	39.903	1.00 17.05
MOTA	1750		21.492	38.550	38.909	1.00 17.79
MOTA			20.127	38.601	39.051	1.00 19.77
MOTA	1751		28.316	39.963	38.843	1.00 19.95
ATOM	1752		29.722	39.829	39.213	1.00 20.42
MOTA	1753		30.157	38.339	39.187	1.00 20.93
MOTA	1754		29.345	37.463	39.506	1.00 20.71
MOTA	1755		29.755	40.369	40.642	1.00 20.70
MOTA	1756		28.588		40.716	1.00 20.76
MOTA	1757		27.528	40.701	39.845	1.00 19.53
MOTA	1758	CD PRO A 231	31.413		38.831	1.00 20.93
MOTA	1759		31.413		38.742	1.00 21.31
MOTA	1760				40.014	
MOTA	1761		31.722 31.431			1.00 20.50
MOTA	1762					1.00 21.35
MOTA	1763		33.398			1.00 22.23
MOTA	176		34.029			1.00 22.23
MOTA			33.533			1.00 21.71
MOTA			31.872			1.00 21.10
ATOM			31.742			
ATOM			30.302			
MOTA			30.045			
MOTA			32.606			
. ATOM	177	1 CG HIS A 233	34.063			
MOTA			34.720			
ATOM			34.993		_	
ATOM			35.994			
ATOM			36.186			
ATOM			29.36			
ATOM		7 CA HIS A 234	27959			
ATOM			27.49			
ATOM			28.02			
ATOM			27.16	9 37.203	3 41.989	1.00 21.52

MOTA	1781	CG	HIS A 234	25.730	37.253	42.374	1.00 21.54	С
MOTA	1782	ND1	HIS A 234	24.769	36.498	41.740	1.00 21.95	N
MOTA	1783	CD2	HIS A 234	25.073	38.028	43.269	1.00 22.67	С
ATOM	1784	CE1	HIS A 234	23.585	36.779	42.254	1.00 22.38	С
ATOM	1785		HIS A 234	23.743	37.700	43.187	1.00 21.91	N
ATOM	1786	N	PRO A. 235	26.551	34.087	42.792	1.00 21.11	N
ATOM	1787	CA	PRO A 235	25.999	32.809	42.338	1.00 21.46	Ċ
	1788	C	PRO A 235	25.461	32.835	40.916	1.00 21.10	č
ATOM					31.802	40.244	1.00 21.10	0
ATOM	1789	0	PRO A 235	25.517				
ATOM	1790	CB	PRO A 235	24.860	32.551	43.325	1.00 21.90	c
ATOM	1791	CG	PRO A 235	25.316	33.240	44.574	1.00 22.00	. C
ATOM	1792	CD	PRO A 235	26.007	34.485	44.100	1.00 21.41	· c
MOTA	1793	N	CYS A 236	24.997	33.989	40.452	1.00 20.41	N
ATOM	1794	CA	CYS A 236	24.456	34.077	39.110	1.00 20.17	С
MOTA	1795	С	CYS A 236	25.503	34.554	38.107	1.00 20.00	С
MOTA	1796	0	CYS A 236	25.180	35.111	37.061	1.00 20.30	0
MOTA	1797	CB	CYS A 236	23.195	34.924	39.090	1.00 19.66	С
MOTA	1798	SG	CYS A 236	21.914	34.209	40.133	1.00 20.71	S
ATOM	1799	N	ASP A 237	26.768	34.311	38.433	1.00 19.87	N
MOTA	1800	CA	ASP A 237	27.857	34.498	37.485	1.00 19.60	C
ATOM	1801	C	ASP A 237	27.459	33.915	36.105	1.00 19.48	C
ATOM	1802	Ö	ASP A 237	26.883	32.834	36.020	1.00 18.94	ō
ATOM	1803	СВ	ASP A 237	29.075	33.789	38.031	1.00 19.20	
ATOM	1804	CG	ASP A 237	30.268	33.842	37.107	1.00 20.58	č
ATOM			ASP A 237		34.871	36.373	1.00 20.58	Õ
	1805			30.477				0
ATOM	1806		ASP A 237	31.070		3,10,,	1.00 13.01	
ATOM	1807	N	ARG A 238	27.749		35.056	1.00 19.85	N
ATOM	1808	CA	ARG A 238	27.459		33.664	1.00 20.90	C
MOTA	1809	С	ARG A 238	26.002		33.247	1.00 20.67	С
MOTA	1810	0	ARG A 238	25.709		32.059	1.00 21.20	0
MOTA	1811	CB	ARG A 238	27.854	32.876	33.319	1.00 21.44	С
ATOM	1812	CG	ARG A 238	29.330	32.585	33.482	1.00 21.04	С
ATOM	1813	CD	ARG A 238	29.710	31.150	33.145	1.00 22.38	С
. ATOM	1814	NE	ARG A 238	29.080	30.243	34.085	1.00 23.86	. N
ATOM	1815	CZ	ARG A 238	27.937	29.584	33.874	1.00 25.81	С
ATOM	1816	NH1	ARG A 238	27.262	29.686	32.712	1.00 24.18	N
MOTA	1817		ARG A 238	27.471		34.849	1.00 27.18	N
ATOM	1818	N	GLN A 239	25.105		34.190	1.00 19.94	N
ATOM	1819	CA	GLN A 239	23.722		33.833	1.00 20.58	C
ATOM	1820	C	GLN A 239	23.535		33.740	1.00 20.50	C
ATOM	1821	Ö	GLN A 239	24.219		34.446	1.00 20.63	Ö
ATOM	1822	СВ	GLN A 239	22.735		34.863	1.00 20.32	Č
	1823		GLN A 239	23.159		35.594	1.00 20.32	č
ATOM	1824	CG	GLN A 239			34.673		C
ATOM		CD						
MOTA	1825		GLN A 239			34.014	1.00 21.22	0
MOTA	1826		2 GLN A 239			34.616		N
MOTA	1827	N	SER A 240			32.900		N
MOTA	1828	CA	SER A 240			32.768		C
MOTA	1829		SER A 240			33.969		С
MOTA	1830		SER A 240					0
MOTA	1831	CB	SER A 240	21.405	38.776			С
ATOM	1832	OG	SER A 240	21.007	40.137	31.454	1.00 21.43	. 0
ATOM	1833	N	GLN A 243				1.00 20.46	Ŋ
ATOM	1834		GLN A 24:					С
ATOM	1835		GLN A 24:					C
ATOM	1836		GLN A 241					0
ATOM	1837		GLN A 24:					. C
MOTA	1838		GLN A 24					· C
ATOM	1839		GLN A 24:					Č
ATOM	1840		1 GLN A 24					o
ATOM	1841		2 GLN A 24					N
AIOH	TOAT	MEN	. GDN A 24.	24.07	, 40.004	50.024	1.00 20.04	IN

ATOM	1842	N	VAL 2			19.557	41.563	33.659	1.00	20.57		N
MOTA	1843	CA	VAL A			18.361	42.229	33.182		20.73		С
MOTA	1844	С	VAL .			17.173	41.309	33.246	1.00	20.69		С
MOTA	1845	0	VAL .			17.244	40.190	32.757		21.13		0
MOTA	1846	CB	VAL :			18.498	42.667	31.712		21.03		С
MOTA	1847		VAL .			17.204	43.377	31.250		20.85		С
MOTA	1848		VAL .			19.723	43.527	31.498		20.71		С
ATOM	1849	N	ASP .			16.071	41.786	33.813		20.62		N
ATOM	1850	CA	ASP .			14.807	41.042	33.788		20.64		С
MOTA	1851	C	ASP			14.148	41.348	32.448		20.94		C
ATOM	1852	0	ASP			13.591	42.438	32.230		19.75		0
ATOM	1853	CB	ASP			13.916	41.471	34.963		20.88		C
MOTA	1854	CG	ASP			12.526	40.894	34.898		21.39		С
ATOM	1855		ASP			12.209	40.153	33.941		23.25		0
ATOM	1856		ASP			11.672	41.130	35.784		23.49		0
MOTA	1857	N	PHE			14.238	40.385	31.541		21.19		N
ATOM ATOM	1858 1859	CA C	PHE PHE			13.717 12.225	40.549 40.916	30.197 30.204		21.56	•	C C
MOTA	1860	0	PHE			11.734	40.516	29.260		22.49 21.85		0
ATOM	1861	CB	PHE			13.940	39.275	29.378		21.85		c
ATOM	1862	CG	PHE			15.316	39.152	28.743		20.87		c
ATOM	1863		PHE			16.457	39.540	29.399		20.74		C
ATOM	1864		PHE			15.446	38.617	27.483		21.00		c
ATOM	1865		PHE			17.691	39.407	28.810		19.77		Č
ATOM	1866	CE2				16.687	38.470	26.890		20.94		Ċ
ATOM	1867	CZ	PHE			17.805	38.881	27.551		20.34		Ċ
MOTA	1868	N	ASP			11.500	40.554	31.259		23.56		N
MOTA	1869	CA	ASP	Α	245	10.072	40.831	31.311	1.00	24.26	•	C
MOTA	1870	С	ASP	Α	245	9.794	42.256	31.814	1.00	24.66		С
MOTA	1871	0	ASP			8.711	42.762	31.607		24.21		0
MOTA	1872	CB	ASP			9.353	39.841	32.222		24.74		С
ATOM	1873	CG	ASP			9.408	38.427	31.721	1.00			C
MOTA	1874		ASP			9.368	38.210	30.493		28.81		0
ATOM	1875		ASP			9.489	37.455	32.498		28.39		0
MOTA	1876	N	ASN ASN			10.758	42.876	32.492		24.80		N C
ATOM ATOM	1877 1878	CA C	ASN			10.605 11.960	44.244 44.902	32.989 33.106	1.00	25.56 25.31		C
ATOM	1879	0	ASN			12.500	45.064	34.205		25.43		0
ATOM	1880	СВ	ASN			9.912	44.285	34.345		26.09		c
ATOM	1881	CG	ASN			9.555	45.716	34.765		29.59		č
MOTA	1882		ASN			9.366	46.598	33.912		32.67		ō
ATOM	1883		ASN			9.468	45.954	36.075		33.42		N
MOTA	1884	N			247	12.525	45.257	31.961		25.08		N
MOTA	1885	CA			247	13.885	45.782	31.911	1.00	24.89		С
ATOM	1886	С			247	13.992	47.144	32.579		24.95		С
MOTA	1887	0			247	13.217	48.049	32.297		24.55		0
MOTA	1888	CB			247	14.182	45.899	30.413		25.05		С
ATOM	1889	CG			247	13.016	45.325	29.702		25.39		C
ATOM	1890	CD			247	11.890	45.184	30.640		25.02		C
MOTA	1891	N			248	14.976	47.267	33.460		24.53		N
ATOM ATOM	1892 1893	CA C			248 248	15.216 16.271	48.489 49.284	34.167 33.389		24.65 24.54		C C
MOTA	1894	0			248	17.472	49.204	33.552		23.15		Ö
ATOM	1895	СВ			248	15.706	48.144	35.564		24.64		c
ATOM	1896	CG			248	15.787	49.343	36.454		26.02		C
MOTA	1897		ASP			16.035	50.466	35.944		26.95		Õ
ATOM	1898		ASP			15.609	49.249	37.684		27.69		ō
ATOM	1899	N			249	15.812	50.181	32.525		24.81		N
ATOM	1900	CA			249	16.720	50.936	31.673		25.45		C
MOTA	1901	С			249	17.573	51.954	32.426		25.90		С
MOTA	1902	0			249	18.585	52.421	31.897		25.80		0

ATOM	1903	СВ	TYR			15.948	51.615	30.544	1.00 25.57	С
ATOM	1904	CG	TYR			15.244	50.651	29.630	1.00 24.58	С
MOTA	1905					15.930	49.624	29.003	1.00 25.44	C
ATOM	1906		TYR			13.890	50.764	29.404	1.00 24.48	C
ATOM	1907		TYR		_	15.276	48.731	28.173	1.00 25.01	C
MOTA	1908	CE2	TYR			13.234	49.892	28.583	1.00 24.43	C
ATOM	1909	CZ	TYR			13.927	48.883	27.969	1.00 24.47	C
ATOM	1910	ОН	TYR			13.252	48.043	27.142 33.660	1.00 25.97	0
ATOM	1911 1912	N	GLU			17.195	52.278 53.190		1.00 26.10	C N
ATOM	1912	CA C	GLU GLU			17.999 19.259	52.492	34.458 34.929	1.00 26.93 1.00 25.85	c
ATOM ATOM	1913	0	GLU			20.329	53.086	34.964	1.00 25.83	0
ATOM	1915	СВ	GLU			17.219	53.740	35.661	1.00 23.30	c
ATOM	1916	CG	GLU			16.021	54.576	35.246	1.00 27.30	č
ATOM	1917	CD	GLU-			15.420	55.366	36.385	1.00 36.85	Ċ
ATOM	1918		GLU			15.945	55.309	37.516	1.00 42.35	Ö
ATOM	1919		GLU			14.422	56.057	36.142	1.00 40.82	ō
ATOM	1920	N	ARG			19.136	51.233	35.315	1.00 24.58	N
ATOM	1921	CA	ARG			20.297	50.502	35.756	1.00 23.76	C
ATOM	1922	C	ARG			21.030	49.909	34.568	1.00 22.91	č
	. 1923	Ö			251	22.242	49.773	34.602	1.00 22.42	Ō
ATOM	1924	СВ			251 .	19.896	49.374	36.696	1.00 24.55	, c
ATOM	1925	CG			251	19.421	49.802	38.077	1.00 25.88	Ċ
ATOM	1926	CD			251	18.894	48.629	38.921	1.00 29.50	Ċ
ATOM	1927	NE			251	19.993	47.764	39.349	1.00 31.63	N
MOTA	1928	CZ			251	19.894	46.467	39.623	1.00 33.13	C
ATOM	1929		ARG			18.736	45.826	39.521	1.00 33.12	N
ATOM	1930	NH2			251	20.978	45.805	39.998	1.00 33.93	N
MOTA	1931	N			252	20.300	49.560	33.515	1.00 21.47	Ŋ
ATOM	1932	CA			252	20.898	48.863	32.379	1.00 21.32	С
ATOM	1933	С			252	20.576	49.552	31.056	1.00 20.68	С
· ATOM	1934	Ō			252	19.934	48.984	30.187	1.00 20.79	0
ATOM	1935	CB			252	20.355	47.434	32.344	1.00 21.09	С
ATOM	1936	CG			252	20.373	46.738	33.690	1.00 20.96	С
ATOM	1937		PHE			21.555	46.560	34.376	1.00 19.28	С
MOTA	1938		PHE			19.207	46.238	34.247.	1.00 21.43	С
MOTA	1939	CE1	PHE	Α	252	21.571	45.891	35.609	1.00 20.54	. C
MOTA	1940	CE2	PHE	Α	252	19.217	45.588	35.488	1.00 22.13	С
ATOM	1941	CZ	PHE	Α	252	20.403	45.414	36.156	1.00 20.96	·C
MOTA	1942	N	PRO	Α	253	21.057	50.767	30.884	1.00 20.56	Ŋ
MOTA	1943	CA	PRO	Α	253	20.658	51.566	29.714	1.00 20.38	Ċ
MOTA	1944	С	PRO	A	253	20.984		28.361	1.00 20.20	C
MOTA	1945	0			253	20,191		27.428	1.00 19.48	0
MOTA	1946	CB			253	21.383		29.928	1.00 19.77	С
MOTA	1947	CG			. 253	22.562		30.895	1.00 20.60	С
ATOM	1948	CD			. 253	21.986		31.782	1.00 20.69	С
ATOM	1949	N			. 254	22.091		28.240	1.00 20.32	N
ATOM	1950	CA			254	22.409		26.938	1.00 20.12	С
MOTA	1951	С			254	21.572		26.554	1.00 19.96	С
MOTA	1952	0			254	21.675		25.441	1.00 19.16	0
ATOM	1953	CB			254	23.893		26.784	1.00 20.06	C
MOTA	1954	CG			254	24.706		26.697	1.00 21.51	C
ATOM	1955				254	25.502		27.598	1.00 23.96	0
ATOM	1956				254	24.514		25.614	1.00 20.38	N
ATOM	1957	N			255	20.724		27.455	1.00 19.81	N
ATOM	1958	CA			255	19.807		27.063	1.00 19.54	C
ATOM	1959	C			255	18.855		25.977	1.00 19.69	. С
ATOM	1960	0			255	18.194		25.274	1.00 19.77	0
ATOM	1961	CB			255	19.023		28.252	1.00 19.22	C
ATOM	1962	CG CD1			255	18.269		27.940	1.00 20.47	C
MOTA	1963	. CD1	. PHE	ı A	255	18.928	43.922	27.736	1.00 20.23	C

MOTA	1964	CD2	PHE .	A :	255	16.909	45.148	27.758	1.00	20.13		C
ATOM	1965	CE1	PHE :	A:	255	18.243	42.786	27.416	1.00	21.65		С
ATOM	1966	CE2	PHE .	A	255	16.227	44.023	27.432	1.00	20.73	•	С
MOTA	1967	CZ	PHE .			16.886	42.842	27.257		22.63		C
ATOM	1968	N	GLN			18.790	48.707	25.841		19.89		N
ATOM	1969	CA	GLN			17.969	49.345	24.794		20.24		Č
ATOM	1970	C	GLN .			18.595	49.160	23.403		19.74		C
ATOM	1971	0	GLN			17.969	49.443	22.384		19.92		0
ATOM	1972	CB	GLN			17.778	50.849	25.095		20.01	_	С
MOTA	1973	CG	GLN			16.736	51.095	26.197		21.20		С
ATOM .	1974	CD	GLN			16.741	52.513	26.764	1.00	22.14		С
ATOM	1975		GLN			15.711	53.195	26.741	1.00	23.01		0
MOTA	1976	NE2	GLN	Α	256	17.874	52.943	27.298	1.00	21.42		N
ATOM	1977	N	ASN	Α	257	· 19.845	48.716	23.385	1.00	19.66		N
MOTA	1978	CA	ASN	Α	257	20.580	48.485	22.155	1.00	20.07		С
ATOM	1979	С	ASN			20.757	47.005	21.811		20.73		C
ATOM	1980	ō	ASN			21.416	46.694	20.823		20.96		Ō
ATOM	1981	CB	ASN			21.969	49.100	22.232		19.17		Č
ATOM	1982	CG	ASN			21.941	50.550	22.635		20.82		Č
												0
ATOM	1983		ASN			22.413	50.902	23.722		21.51		
ATOM	1984		ASN			21.396	51.407	21.763		16.92		N
MOTA	1985	N	VAL			20.190	46.098	22.596		21.59		N
ATOM	1986	CA	VAL			20.410	44.660	22.347		23.34		С
MOTA	1987	C	VAL	Α	258	19.671	44.172	21.112	1.00	23.85		С
MOTA	1988	0	VAL	Α	258	18.549	44.611	20.818	1.00	24.10		0
ATOM	1989	CB	VAL	Α	258	20.015	43.806	23.573	1.00	23.68		С
ATOM	1990	CG1	VAL	Α	258	18.507	43.720	23.685	1.00	24.12		С
ATOM	1991	CG2	VAL	Α	258	20.570	42.436	23.445	1.00	28.30		С
MOTA	1992	N	VAL			20.314	43.286	20.360		24.47		N
ATOM	1993	CA	VAL			19.705	42.721	19.154		24.91		C
ATOM	1994	C	VAL			20.004	41.215	19.140		24.93		Ċ
ATOM	1995	Ö	VAL			21.152	40.829	19.119		25.32		ŏ
												c
ATOM	1996	CB	VAL			20.281	43.362	17.895		24.88		
MOTA	1997		VAL			19.667	42.738	16.670		26.38		С
MOTA	1998		VAL			20.051	44.869	17.909		24.83		С
MOTA	1999	N			260	18.974	40.381	19.186		25.06		N
MOTA	2000	CA			260	19.166	38.944	19.232		25.64		С
MOTA	2001	С	GLY	Α	260	19.076	38.221	17.887		25.42		С
MOTA	2002	0	\mathtt{GLY}	Α	260	18.679	38.796	16.869	. 1.00	25.77		0
MOTA	2003	N	TYR	Α	261	19.497	36.965	17.907	1.00	25.04		N
ATOM	2004	CA	TYR	Α	261	19.380	36.049	16.792	1.00	25.30		С
ATOM	2005	С	TYR	Α	261	18.428	34.973	17.328	1.00	24.63		C
ATOM	2006	0			261	18.676	34.417	18.392		24.77		0
ATOM	2007	CB			261	20.729	35.414	16.482		25.84		С
ATOM	2008	CG			261	21.750	36.315	15.825		28.57		C
ATOM	2009		TYR			21.821	36.423	14.447		34.41		Ċ
MOTA	2010		TYR			22.631	37.049	16.574		29.87		Č
ATOM						22.752				35.64		c
	2011		TYR				37.255	13.838				
MOTA	2012				261	23.576	37.852	15.986		32.26		C
MOTA	2013	CZ			261	23.644	37.949	14.623		34.92		C
MOTA	2014	OH			261	24.582	38.772	14.047		38.39		0
MOTA	2015	N			262	17.325	34.698	16.658		23.64		N
ATOM	2016	CA			262	16.376	33.758	17.244	1.00	24.03		. С
MOTA	2017	C	GLU	Α	262	15.933	32.660	16.306		23.15		С
MOTA	2018	0	GLU	A	262	16.063	32.766	15.078	1.00	22.51		0
MOTA	2019	CB			262	15.172	34.482	17.861		24.11		С
MOTA	2020	CG			262	13.899	34.502	17.057		26.35		C
ATOM	2021	CD			262	12.744	35.177	17.785		27.98		Ċ
ATOM	2022		. GLU			12.743	36.415	17.872		27.19		ŏ
ATOM	2023		GLU			11.818	34.476	18.254		29.21		Ö
MOTA	2024	N			263	15.455	31.587	16.234		22.58		N
111011	2023		T 111/		200	10.400	31.307	10.91	1.00			74

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ATOM	2025	CA	THR A		14.939	30:458	16.170	1.00 22.5	52
ATOM	2026	С	THR A		14.047	29.617	17.076	1.00 22.4	18
MOTA	2027	0	THR A		14.107	29.712	18.313	1.00 22.3	
ATOM	2028	CB	THR A		16.117	29.607	15.659	1.00 22.5	55
MOT	2029		THR A		15.665	28.666	14.675	1.00 22.2	
MOTA	2030		THR A		16.693	28.743	16.770	1.00 22.7	
MOTA	2031	N	VAL A		13.208	28.797	16.472	1.00 21.6	
ATOM	2032	CA	VAL A		12.453	27.860	17.263	1.00 22.4	
ATOM	2033	С	VAL A	264	12.871	26.474	16.837	1.00 22.	
MOTA	2034	0	VAL A	264	12.779	26.134	15.673	1.00 22.7	
ATOM	2035	CB	VAL A		10.964	28.027	17.087	1.00 23.0	
ATOM	2036	CG1	VAL A	264	10.234	26.805	17.643	1.00 23.6	
ATOM'	2037	CG2	VAL A	264	10.499	29.344	17.767	1.00 22.	
ATOM	2038	N	VAL A		13.389	25.695	17.777	1.00 22.9	
ATOM	2039	CA	VAL A		13.779	24.329	17.458	1.00 23.0	
ATOM	2040	С	VAL A	265	12.738	23.317	17.886	1.00 22.8	
ATOM	2041	0	VAL A	265	12.105	23.473	18.932	1.00 23.0	
ATOM	2042	CB	VAL A		15.143	23.937	18.075	1.00 22.9	
MOTA	2043		VAL A		16.243	24.745	17.404	1.00 23.6	
MOTA	2044	CG2	VAL A	265	15.169	24.122	19.592	1.00 22.9	
MOTA	2045	N	GLY A	266	12.574	22.290	17.056	1.00 21.7	
MOTA	2046	CA	GLY A		11.683	21.178	17.355	1.00 21.9	
MOTA	2047	С	GLY A	266	12.376	19.826	17.263	1.00 20.9	
ATOM	2048	0	GLY A		13.562	19.757	16.999	1.00 20.6	
MOTA	2049	N	PRO A	267	11.643	18.737	17.461	1.00 21.2	
MOTA	2050	CA	PRO A		12.253	17.403	17.427	1.00 20.6	
MOTA	2051	С	PRO A		13.126	17.183	16.203	1.00 20.0	
ATOM	2052	0	PRO A	267		17.371	15.081	1.00 19.3	
MOTA	2053	CB	PRO A	267	11.039	16.463	17.379	1.00 21.2	
ATOM	2054	CG	PRO A	267	9.970	17.202	18.037	1.00 22.8	
ATOM	2055	CD	PRO A	267	10.188	18.676	17.710	1.00 21.6	
ATOM	2056	N	GLY A	268	14.376	16.787	16.411	1.00 20.3	
MOTA	2057	CA	GLY A	268	15.278	16.518	15.305	1.00 19.9	
ATOM	2058	С	GLY A		16.256	17.627	14.993	1.00 20.5	
MOTA	2059	0	GLY A		17.277	17.400	14.311	1.00 21.6	
MOTA	2060	N	ASP A		15.965	18.831	15.477	1.00 19.8	
ATOM	2061	CA	ASP A	269	16.818	19.977	15.217	1.00 19.7	
MOTA	2062	С	ASP A	269	17.970	20.003	16.215	1.00 19.6	
ATOM	2063	0	ASP A		17.811	19.625	17.377	1.00 18.7	
MOTA	2064	CB	ASP A	269	16.032	21.288	15.386	1.00 19.9	
MOTA	2065	CG	ASP A	269	14.916	21.464	14.374	1.00 20.9	
ATOM	2066	OD1	ASP A	269	14.935	20.842	13.287	1.00 22.1	
MOTA	2067	OD2	ASP A	269	13.987	22.259	14.576	1.00 23.2	
ATOM	2068	N	VAL A	270	19.116	20.481	15.746	1.00 19.5	
MOTA	2069	CA	VAL A	270	20.276	20.700	16.595	1.00 19.5	
ATOM	2070	С	VAL A	270	20.747	22.137	16.444	1.00 19.3	
MOTA	2071	Ο.	VAL A	270	21.033	22.594	15.352	1.00 19.7	
ATOM	2072	CB	VAL A		21.404	19.776	16.215	1.00 19.5	
ATOM	2073		VAL A		22.646	20.154	16.966	1.00 20.0	
ATOM	2074	CG2	VAL A	270	21.001	18.342	16.535	1.00 19.4	
ATOM	2075	N	LEU A	271	20.786	22.870	17.539	1.00 19.3	
ATOM	2076	CA	LEU A	271	21.263	24.229	17.501	1.00 19.0	
MOTA	2077	С	LEU A		22.677	24.272	18.036	1.00 19.1	
MOTA	2078	0	LEU A	271	22.961	23.787	19.130	1.00 18.7	
MOTA	2079	CB	LEU A		20.376	25.120	18.331	1.00 19.9	
MOTA	2080	CG	LEU A		20.892	26.549	18.573	1.00 20.1	
ATOM	2081		LEU A	271	21.011	27.358	17.296	1.00 19.4	
MOTA	2082		LEU A		19.979	27.245	19.555	1.00 20.2	
MOTA	2083	N	TYR A		23.582	24.818	17.244	1.00 20.2	
MOTA	2084	CA	TYR A		24.924	25.051	17.718	1.00 19.7	
MOTA	2085.	С	TYR A	272	24.914	26.360	18.483	1.00 19.6	

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ATOM	2086 O TYR A 272	24.646	27.395		1.00 20.44
ATOM	2087 CB TYR A 272	25.908	25.172	16.547	1.00 19.86
	2088 CG TYR A 272	27.293	25.654	16.962	1.00 21.59
ATOM	2089 CD1 TYR A 272	27.952	25.093	18.048	1.00 22.02
MOTA	_	27.936	26.668		1.00 20.87
MOTA	- ·	29.214	25.522		1.00 19.87
MOTA	2091 CE1 TYR A 272		27.098		1.00 20.88
MOTA	2092 CE2 TYR A 272	29.200			1.00 21.07
MOTA	2093 CZ TYR A 272	29.834	26.517		
MOTA	2094 OH TYR A 272	31.091	26.937		1.00 18.93
MOTA	2095 N ILE A 273	25.210	26.308		1.00 19.80
ATOM	2096 CA ILE A 273	25.342	27.500		1.00 20.12
ATOM	2097 C ILE A 273	26.837	27.683	20.883	1.00 20.39
ATOM	2098 O ILE A 273	27.393	27.000	21.760	1.00 19.88
ATOM	2099 CB ILE A 273	24.576	27.366	21.901	1.00 19.72
MOTA	2100 CG1 ILE A 273	23.111	27.045	21.624	1.00 20.57
	2100 CG1 IDE N 273	24.661	28.695	22.696	1.00 20.99
ATOM		22.296	26.797	22.876	1.00 20.93
ATOM		27.487	28.611	20.182	1.00 20.23
MOTA	2103 N PRO A 274	28.938	28.743	20.326	1.00 21.16
MOTA	2104 CA PRO A 274		29.264	21.704	1.00 21.39
ATOM	2105 C PRO A 274	29.289	30.027	22.317	1.00 20.89
MOTA	2106 O PRO A 274	28.520			1.00 20.03
MOTA	2107 CB PRO A 274	29.353	29.757	19.230	
MOTA	2108 CG PRO A 274	28.089	30.056	18.410	1.00 21.22
MOTA	2109 CD PRO A 274	26.919	29.621	19.282	1.00 20.51
MOTA	2110 N MET A 275	30.450	28.831	22.180	1.00 21.53
ATOM	2111 CA MET A 275	30.953	29.207	23.479	1.00 22.30
MOTA	2112 C MET A 275	30.920	30.734	23.636	1.00 21.94
ATOM	2113 O MET A 275	31.160	31.442	22.675	1.00 20.78
ATOM	2114 CB MET A 275	32.367	28.695	23.589	1.00 23.06
MOTA	2115 CG MET A 275	32.937	28.734	24.966	1.00 27.00
ATOM	2116 SD MET A 275	34.545	27.926	24.991	1.00 33.74
	2117 CE MET A 275	35.263	28.479	23.499	1.00 32.50
MOTA		30.583	31.211	24.832	1.00 21.96
ATOM		30.485	32.656	25.138	1.00 23.15
ATOM		29.256	33.365	24.546	1.00 22.39
MOTA		28.989	34.496	24.899	1.00 22.58
MOTA	2121 O TYR A 276	31.776		24.760	
MOTA	2122 CB TYR A 276		33.136		1.00 28.82
MOTA	2123 CG TYR A 276	32.904			1.00 32.73
MOTA	2124 CD1 TYR A 276	32.940			1.00 35.83
MOTA	2125 CD2 TYR A 276	33.935			1.00 35.05
ATOM	2126 CE1 TYR A 276	33.956		27.864	1.00 33.50
MOTA	2127 CE2 TYR A 276	34.975			
MOTA	2128 CZ TYR A 276	34.958			1.00 38.60
MOTA	2129 OH TYR A 276	35.951			1.00 45.18
MOTA	2130 N TRP A 277	28.488			1.00 21.71
MOTA	2131 CA TRP A 277	27.281			1.00 21.24
MOTA	2132 C TRP A 277	26.184			1.00 20.90
ATOM	2133 O TRP A 277	25.914	32.217		1.00 21.96
MOTA	2134 CB TRP A 277		32.711	21.856	1.00 21.01
MOTA	2135 CG TRP A 277			20.670	1.00 19.98
ATOM				20.462	1.00 17.90
MOTA					
MOTA					
ATOM					
MOTA	1 2146 C TRP A 278	23.26	33.78	, 24.141	. 1.00 13.33

ATOM	2147	0	TRP	A	278	23.08	3 33.758	23.538	1.00 20.	42		,
ATOM	2148	CB			. 278	24.02	5 35.999		1.00 20.			Č
ATOM	2149	,CG			278	25.03			1.00 20.			ì
ATOM ATOM	2150				278	26.07		25.519	1.00 19.	63		Ò
ATOM	2151 2152				278	25.09			1.00 19.	59		(
ATOM	2152				278	26.77		26.469	1.00 20.			1
ATOM	2154				278	26.19		27.699	1.00 20.			(
ATOM	2155				278	24.318 26.52		28.601	1.00 20.			(
ATOM	2156				278	24.66		28.951	1.00 20.			(
ATOM	2157				278	25.75		29.849 30.011	1.00 23.			(
MOTA	2158	N			279	22.46		25.591	1.00 20. 1.00 19.			(
MOTA	2159	CA			279	21.26		25.122	1.00 19.			F
. ATOM	2160	С			279	20.20		26.192	1.00 20.			
ATOM	2161	0			27,9	20.47		27.370	1.00.20.			
ATOM	2162	CB			279	21.54		24.604	1.00 20.			Č
ATOM ATOM	2163	CG			279	22.34		25.528	1.00 21.			Ċ
ATOM	2164 2165				279	23.720		25.608	1.00 23.			Ŋ
ATOM	2166		HIS		279	21.988		26.371	1.00 23.	96		C
ATOM	2167	NE2	HIS	Δ	279	24.175		26.449				C
ATOM	2168	N			280	23.144 18.994		26.940	1.00 23.			N
ATOM	2169	CA			280	17.742		25.711 26.441	1.00 20.			Ŋ
MOTA	2170	С			280	16.91		25.793	1.00 21.3 1.00 21.4		-	
ATOM	2171	0			280	16.749		24.580	1.00 21.			
ATOM	2172	CB			280	17.099	34.124	26.224	1.00 21.0			(
ATOM	2173	CG			280	15.632	34.168	26.489	1.00 21.			Ċ
ATOM	2174		HIS			15.096		27.571	1.00 22.			N
ATOM ATOM	2175 2176		HIS			14.581		25.802	1.00 22.			C
ATOM	2177	MES	HIS HIS	A	280	13.779	•	27.546	1.00 23.2			C
ATOM	2178	N			281	13.441	•	26.482	1.00 23.0			N
ATOM	2179	CA			281	16.367 15.649		26.584	1.00 22.3			N
ATOM	2180	С			281	14.304		26.040 26.722	1.00 22.3			C
MOTA	2181	0			281	14.216		27.945	1.00 22.7 1.00 22.7			0
MOTA	2182	CB			281	16.527		26.189	1.00 22.9			C
ATOM	2183	CG1	ILE			17.771	28.504	25.305	1.00 24.9		-	C
ATOM	2184		ILE			15.770	-	25.771	1.00 21.0			Ċ
ATOM ATOM	2185	CD1			281	18.795		25.554	1.00 27.3	31		C
ATOM	2186 2187	N CA			282 282	13.252		25.920	1.00 22.9			N
ATOM	2188	C	GLU			11.903		26.458	1.00 23.3			С
ATOM	2189	Ö	GLU			11.101 11.092		25.769	1.00 22.5			С
ATOM	2190	CB	GLU			11.144		24.549 26.393	1.00 21.7			0
MOTA	2191	CG	GLU			10.830		25.009	1.00 23.4 1.00 25.7			C
ATOM	2192	CD	GLU	Α	282	10.281		25.023	1.00 25.7			C
ATOM	2193	OE1	GLU	A	282	10.898		25.665	1.00 27.4			0
ATOM	2194		GLU			9.241	32.740	24.391	1.00 26.0			0
ATOM ATOM	2195	N	SER			10.456		26.588	1.00 22.4			N
ATOM	2196 2197	CA	SER			9.570		26.103	1.00 23.0			С
ATOM	2197	С 0	SER			8.256		25.753	1.00 23.5			С
ATOM	2199	СВ	SER SER			7.685		26.584	1.00 24.1			0
ATOM	2200	OG	SER			9.346 10.496		27.188	1.00 22.5			С
ATOM	2201	N	LEU			7.763		27.345	1.00 22.6			0
ATOM	2202	CA	LEU			6.581		24.541 24.070	1.00 24.0 1.00 24.8			N
ATOM	2203	С	LEU	Α	284	5.386		25.004	1.00 24.8			C
ATOM	2204	0	LEU	Α	284	5.098		25.602	1.00 24.5			0
ATOM	2205	CB	LEU			6.161	26.947	22.682	1.00 25.0			C
ATOM ATOM	2206	CG	LEU	A	284	7.185		21.555	1.00 26.4	6		c
ALON	2207	CDI	LEU	A	284	6.475	27.236	20.215	1.00 28.2	9		C

ATOM 2208 N LEU A 284			* DIT 7 204	8.123	28.188	21.775 1	00 26.10
ATOM 2210 CA LBU A 285							
ATOM 2211 C LEU A 285							
ATOM 2212 C LEU A 285	MOTA						
ATOM 2213 CB LEU A 285 3.925 31.078 26.397 1.00 24.79 ATOM 2215 CDI LEU A 285 3.298 32.434 25.954 1.00 26.02 ATOM 2216 CDZ LEU A 285 3.298 32.434 25.954 1.00 26.02 ATOM 2217 N ASN A 286 1.867 26.815 26.173 1.00 25.20 ATOM 2218 CA ASN A 286 1.867 26.815 26.173 1.00 25.20 ATOM 2219 C ASN A 286 1.817 24.7991 24.742 1.00 25.20 ATOM 2219 C ASN A 286 1.317 24.7991 24.742 1.00 25.23 ATOM 2221 CB ASN A 286 -0.319 26.599 25.124 1.00 26.54 ATOM 2221 CB ASN A 286 -0.319 26.599 25.124 1.00 26.54 ATOM 2222 CG ASN A 286 -0.319 26.599 25.124 1.00 26.54 ATOM 2224 NDZ ASN A 286 -0.397 27.546 26.109 1.00 29.40 ATOM 2224 NDZ ASN A 286 -0.397 27.546 26.109 1.00 29.40 ATOM 2224 NDZ ASN A 286 -0.397 27.546 26.109 1.00 29.40 ATOM 2224 NDZ ASN A 286 -0.393 28.843 25.821 1.00 33.58 ATOM 2226 CA GLY A 287 3.243 23.518 23.863 1.00 24.10 ATOM 2227 C GLY A 287 3.243 23.518 23.863 1.00 24.10 ATOM 2228 O GLY A 287 3.524 22.167 24.487 1.00 23.380 ATOM 2228 O GLY A 287 4.110 21.301 23.838 1.00 24.10 ATOM 2229 N GLY A 288 3.360 20.730 26.439 1.00 23.24 ATOM 2230 CA GLY A 288 3.360 20.730 26.439 1.00 23.24 ATOM 2231 C GLY A 288 3.360 20.730 26.439 1.00 23.24 ATOM 2233 N ILE A 289 5.220 19.539 27.462 1.00 23.36 ATOM 2233 N ILE A 289 5.220 19.539 27.462 1.00 23.36 ATOM 2233 N ILE A 289 5.220 19.539 27.462 1.00 23.36 ATOM 2234 CA ILE A 289 7.601 19.374 26.874 1.00 23.36 ATOM 2237 CB ILE A 289 7.601 19.374 26.874 1.00 23.36 ATOM 2237 CB ILE A 289 7.324 18.958 25.755 1.00 23.68 ATOM 2237 CB ILE A 289 7.324 18.958 25.755 1.00 23.69 ATOM 2240 CD ILE A 289 7.324 18.958 25.755 1.00 23.69 ATOM 2240 CD ILE A 289 7.601 19.374 26.874 1.00 23.28 ATOM 2237 CB ILE A 289 7.601 19.374 26.874 1.00 23.29 ATOM 2240 CD ILE A 289 7.601 19.374 26.874 1.00 23.69 ATOM 2237 CB ILE A 289 7.324 18.958 25.755 1.00 23.69 ATOM 2240 CD ILE A 289 7.601 19.374 26.8774 1.00 20.56 ATOM 2240 CD ILE A 289 7.601 19.374 26.8774 1.00 20.56 ATOM 2240 CD ILE A 291 1.100 24.68 ATOM 2240 CD ILE A 291 1.100 24.68 ATOM 2240 CD ILE A 291 1.100 24.68 ATOM 2240 CD ILE A 291 1.2598 1.993 27.26.93	ATOM						
ATOM 2214 CG LEU A 285 3.895 31.078 26.397 1.00 25.19 ATOM 2215 CDL LEU A 285 3.298 32.434 25.954 1.00 26.02 ATOM 2216 CDZ LEU A 285 3.925 30.999 27.898 1.00 26.27 ATOM 2218 CA ASN A 286 1.867 25.848 25.730 1.00 25.25 ATOM 2218 CA ASN A 286 0.867 25.848 25.730 1.00 25.25 ATOM 2219 C ASN A 286 1.371 24.791 24.742 1.00 25.25 ATOM 2210 CB ASN A 286 -0.319 26.599 25.124 1.00 25.23 ATOM 2221 CB ASN A 286 -0.319 26.599 25.124 1.00 26.54 ATOM 2222 CB ASN A 286 -0.319 26.599 25.124 1.00 26.54 ATOM 2223 ODI ASN A 286 -0.957 27.546 26.109 1.00 29.40 ATOM 2223 ODI ASN A 286 -0.957 27.546 26.109 1.00 29.40 ATOM 2223 ODI ASN A 286 -0.893 28.843 25.821 1.00 33.58 ATOM 2225 N GLY A 287 2.669 24.487 24.774 1.00 24.55 ATOM 2226 CA GLY A 287 3.524 22.167 24.487 1.00 24.55 ATOM 2227 C GLY A 287 3.524 22.167 24.487 1.00 23.80 ATOM 2229 N GLY A 288 3.100 21.971 25.734 1.00 23.30 ATOM 2230 CA GLY A 288 3.360 20.730 28.838 1.00 24.10 ATOM 2231 C GLY A 288 3.100 21.971 25.734 1.00 23.32 ATOM 2232 C GLY A 288 4.089 20.673 26.903 1.00 23.24 ATOM 2233 C GLY A 288 4.089 20.673 26.903 1.00 23.24 ATOM 2233 C GLY A 288 4.089 20.673 26.903 1.00 23.24 ATOM 2233 C GLY A 288 4.089 20.673 26.903 1.00 23.39 ATOM 2238 C ILE A 289 7.304 18.958 25.755 1.00 24.68 ATOM 2238 C ILE A 289 7.324 18.958 25.755 1.00 24.68 ATOM 2238 C ILE A 289 7.324 18.958 25.755 1.00 24.68 ATOM 2238 C ILE A 289 7.324 18.958 25.755 1.00 23.69 ATOM 2240 C DI ILE A 289 7.324 18.958 25.755 1.00 23.99 ATOM 2241 N THR A 290 1.0461 21.775 26.053 1.00 29.73 ATOM 2240 C DI ILE A 289 7.324 18.958 25.755 1.00 29.73 ATOM 2240 C DI ILE A 289 7.324 18.958 25.755 1.00 29.73 ATOM 2240 C DI ILE A 289 7.324 18.958 25.755 1.00 29.73 ATOM 2240 C DI ILE A 289 7.324 18.958 25.755 1.00 29.73 ATOM 2240 C DI ILE A 289 7.324 18.958 25.755 1.00 29.73 ATOM 2240 C DI ILE A 289 7.324 18.958 25.755 1.00 29.73 ATOM 2240 C DI ILE A 289 7.324 18.958 25.755 1.00 29.73 ATOM 2240 C DI ILE A 289 7.324 18.958 25.755 1.00 29.73 ATOM 2240 C DI ILE A 289 7.324 18.930 20.910 27.910 1.00 29.44 ATOM 2255 C B ILE A 291	MOTA						
AROM 2215 CD1 LEU A 285 3.298 32.434 25.954 1.00 26.02 AROM 2216 CD2 LEU A 285 3.925 30.999 27.898 1.00 26.02 AROM 2217 N ASN A 286 1.867 26.815 26.173 1.00 25.20 AROM 2219 C ASN A 286 1.371 24.791 24.742 1.00 25.23 AROM 2210 C ASN A 286 1.371 24.791 24.742 1.00 25.23 AROM 2211 CB ASN A 286 0.594 24.267 23.955 1.00 24.38 AROM 2221 CB ASN A 286 -0.319 26.599 25.124 1.00 25.23 AROM 2221 CB ASN A 286 -0.319 26.599 25.124 1.00 25.23 AROM 2222 CG ASN A 286 -0.357 27.546 26.109 1.00 29.40 AROM 2222 ND ASN A 286 -0.893 28.843 25.821 1.00 33.49 AROM 2224 ND2 ASN A 286 -0.893 28.843 25.821 1.00 33.58 AROM 2224 ND2 ASN A 286 -0.893 28.843 25.821 1.00 33.58 AROM 2226 CA GLY A 287 3.524 22.167 24.487 1.00 23.36 AROM 2227 C GLY A 287 3.524 22.167 24.487 1.00 23.36 AROM 2228 O GLY A 287 3.524 22.167 24.487 1.00 23.32 AROM 2229 N GLY A 287 3.524 22.167 24.487 1.00 23.32 AROM 2230 CA GLY A 288 3.360 20.730 26.439 1.00 24.10 AROM 2231 C GLY A 288 3.360 20.730 26.439 1.00 23.24 AROM 2232 C GLY A 288 3.360 20.730 26.439 1.00 23.24 AROM 2233 N LE A 289 5.200 19.539 27.462 1.00 23.36 AROM 2233 N LE A 289 7.001 19.374 26.874 1.00 23.38 AROM 2236 C GLY A 288 5.548 21.646 26.741 1.00 23.36 AROM 2237 C B LE A 289 7.001 19.374 26.874 1.00 23.38 AROM 2238 C GL LE A 289 7.001 19.374 26.874 1.00 23.38 AROM 2239 C GLY A 288 5.548 21.646 26.741 1.00 23.39 AROM 2230 C R LE A 289 7.001 19.374 26.874 1.00 23.28 AROM 2231 C R LE A 289 7.001 19.374 26.874 1.00 23.28 AROM 2232 C R LE A 289 7.001 19.374 26.874 1.00 23.29 AROM 2234 C R LE A 289 7.001 19.374 26.874 1.00 23.29 AROM 2235 C LIE A 289 7.001 19.374 26.874 1.00 23.28 AROM 2236 C R LIE A 289 7.001 19.374 26.874 1.00 23.29 AROM 2237 C R LIE A 289 7.001 19.374 26.874 1.00 20.26.90 AROM 2240 C R LIE A 289 7.001 19.374 26.874 1.00 20.26.90 AROM 2240 C R LIE A 289 7.001 19.374 26.874 1.00 20.26.90 AROM 2240 C R LIE A 289 7.001 19.376 26.493 1.00 29.37 AROM 2240 C R HR A 290 19.304 19.708 26.695 1.00 19.39 AROM 2240 C R HR A 290 19.304 19.709 27.901 19.00 20.01 AROM 2240 C R HR A 290 19.004 19.70	MOTA						
ATOM 2216 CD2 LEU A 285	MOTA						
ATOM 2217 N ASN A 286	ATOM						
ATOM 2218 CA ASN A 286	MOTA						
ATOM 2219 C ASN A 286	MOTA						
ATOM 2220 O ASN A 286	MOTA						
ATOM 2221 CG ASN A 286	ATOM.	2219 C					
ATOM 2221 CG ASN A 286	MOTA	2220 O					
ATOM 2223 OD1 ASN A 286	MOTA	2221 CB					
ATOM 2224 ND2 ASN A 286	ATOM						
ATOM 2225 N GLY A 287	MOTA						
ATOM 2225 N GLY A 287		2224 ND					
ATOM 2226 CA GLY A 287		2225 N					
ATOM 2227 C GLY A 287							
ATOM 2228 O GLY A 287			GLY A 287				
ATOM 2239 N GLY A 288 3.100 21.971 25.734 1.00 23.32 ATOM 2231 C GLY A 288 4.808 20.673 26.493 1.00 23.24 ATOM 2231 C GLY A 288 5.548 21.646 26.903 1.00 23.36 ATOM 2233 N ILE A 289 5.220 19.539 27.462 1.00 23.36 ATOM 2235 C ILE A 289 7.601 19.374 26.874 1.00 23.36 ATOM 2235 C ILE A 289 7.601 19.374 26.874 1.00 23.28 ATOM 2235 C ILE A 289 7.601 19.374 26.874 1.00 23.28 ATOM 2237 CB ILE A 289 6.571 19.406 27.983 1.00 23.99 ATOM 2237 CB ILE A 289 7.601 19.374 26.874 1.00 23.28 ATOM 2238 CG1 ILE A 289 6.750 18.123 28.817 1.00 23.68 ATOM 2239 CG2 ILE A 289 6.819 16.912 27.901 1.00 26.90 ATOM 2240 CD1 ILE A 289 7.294 15.640 28.613 1.00 25.75 ATOM 2241 N THR A 290 8.811 19.790 27.210 1.00 22.42 ATOM 2242 CA THR A 290 8.811 19.790 27.210 1.00 21.38 ATOM 2243 C THR A 290 11.030 18.880 26.774 1.00 20.56 ATOM 2244 O THR A 290 11.030 18.880 26.774 1.00 20.56 ATOM 2244 CG2 THR A 290 11.030 18.880 26.774 1.00 20.56 ATOM 2244 O THR A 290 11.041 18.775 18.296 25.841 1.00 19.36 ATOM 2247 CG2 THR A 290 10.823 21.761 27.308 1.00 21.70 ATOM 2248 N ILE A 291 11.757 18.296 25.841 1.00 19.36 ATOM 2249 CA ILE A 291 11.757 18.296 25.841 1.00 19.36 ATOM 2250 C ILE A 291 11.757 18.296 25.841 1.00 19.36 ATOM 2250 CB ILE A 291 11.757 18.296 25.841 1.00 19.36 ATOM 2250 CB ILE A 291 11.757 18.296 25.841 1.00 19.36 ATOM 2250 CB ILE A 291 11.757 18.296 25.841 1.00 19.36 ATOM 2255 CD1 ILE A 291 11.758 15.609 27.044 1.00 20.08 ATOM 2255 CD ILE A 291 13.873 15.214 26.937 1.00 21.76 ATOM 2255 CD ILE A 291 13.873 15.214 26.937 1.00 20.17 ATOM 2256 CB ILE A 291 13.873 15.214 26.937 1.00 20.08 ATOM 2257 CB ILE A 291 13.873 15.214 26.937 1.00 19.18 ATOM 2258 C THR A 292 15.559 20.724 24.889 1.00 19.18 ATOM 2250 CB ILE A 291 13.873 15.214 26.937 1.00 19.73 ATOM 2250 CB ILE A 291 13.873 15.214 26.937 1.00 19.73 ATOM 2250 CB ILE A 291 13.873 15.214 26.937 1.00 19.79 ATOM 2250 CB ILE A 291 13.873 15.214 26.937 1.00 19.81 ATOM 2250 CB ILE A 291 13.873 15.214 26.937 1.00 19.18 ATOM 2255 CB ILE A 291 13.873 15.214 26.937 1.00 19.19 19.19 ATOM 2256 CB ILE A 2			GLY A 287				
ATOM 2230 CA GLY A 288 3.360 20.730 26.439 1.00 23.24 ATOM 2231 C GLY A 288 4.808 20.673 26.903 1.00 23.49 ATOM 2233 N ILE A 289 5.548 21.646 26.741 1.00 22.86 ATOM 2233 N ILE A 289 5.220 19.539 27.462 1.00 23.36 ATOM 2235 C ILE A 289 7.601 19.374 26.874 1.00 23.99 ATOM 2235 C ILE A 289 7.601 19.374 26.874 1.00 23.28 ATOM 2236 O ILE A 289 7.324 18.958 25.755 1.00 23.68 ATOM 2237 CB ILE A 289 6.819 16.912 27.901 1.00 24.68 ATOM 2238 CG1 ILE A 289 6.819 16.912 27.901 1.00 24.68 ATOM 2230 CG2 ILE A 289 5.648 17.983 29.885 1.00 29.37 ATOM 2241 N THR A 290 8.811 19.790 27.210 1.00 29.37 ATOM 2242 CA THR A 290 9.904 19.768 26.264 1.00 29.37 ATOM 2244 O THR A 290 11.030 18.880 26.774 1.00 20.56 ATOM 2244 C OFT THR A 290 11.030 18.880 26.774 1.00 20.56 ATOM 2244 C OFT THR A 290 11.243 18.743 27.986 1.00 19.81 ATOM 2244 C OFT THR A 290 10.461 21.175 26.053 1.00 20.15 ATOM 2247 CG2 THR A 290 9.405 22.108 25.460 1.00 21.76 ATOM 2248 N ILE A 291 11.757 18.296 25.460 1.00 21.76 ATOM 2249 N ILE A 291 11.757 18.296 25.286 1.00 19.31 ATOM 2250 C ILE A 291 13.862 17.761 25.286 1.00 19.81 ATOM 2250 C ILE A 291 13.862 17.761 25.882 1.00 19.81 ATOM 2255 CD1 ILE A 291 13.862 17.762 24.683 1.00 20.08 ATOM 2255 CD1 ILE A 291 13.862 17.762 24.683 1.00 20.15 ATOM 2256 C ILE A 291 13.863 17.691 25.555 1.00 19.81 ATOM 2256 C ILE A 291 13.863 17.691 25.555 1.00 19.73 ATOM 2256 CB ILE A 291 13.863 17.691 25.555 1.00 19.81 ATOM 2255 CD1 ILE A 291 13.863 17.761 24.863 1.00 19.81 ATOM 2255 CD1 ILE A 291 13.863 17.762 24.881 1.00 19.77 ATOM 2256 CB ILE A 291 13.863 17.762 24.881 1.00 19.78 ATOM 2256 CB ILE A 291 13.863 17.762 24.889 1.00 19.79 ATOM 2256 CB ILE A 291 13.863 17.762 24.889 1.00 19.79 ATOM 2256 CB ILE A 291 13.863 17.762 24.889 1.00 19.79 ATOM 2256 CB ILE A 291 13.863 17.762 24.889 1.00 19.79 ATOM 2256 CB ILE A 291 13.863 17.762 24.889 1.00 19.81 ATOM 2256 CB ILE A 291 13.863 17.762 24.889 1.00 19.79 ATOM 2256 CB ILE A 291 17.667 17.797 24.882 1.00 19.75 ATOM 2256 CB ILE A 291 17.667 17.797 24.893 1.00 20.21 ATOM 2256 CB ILE A 291			GLY A 288				
ATOM 2231 C GLY A 288			GLY A 288	3.360			
ATOM 2232 O GLY A 288 5.548 21.646 26.741 1.00 22.36 ATOM 2233 N ILE A 289 5.220 19.539 27.462 1.00 23.36 ATOM 2235 C ILE A 289 7.601 19.374 26.874 1.00 23.28 ATOM 2236 O ILE A 289 7.324 18.958 25.755 1.00 23.68 ATOM 2237 CB ILE A 289 6.750 18.123 28.817 1.00 24.68 ATOM 2238 CG1 ILE A 289 6.819 16.912 27.901 1.00 26.90 ATOM 2239 CG2 ILE A 289 5.648 17.983 29.885 1.00 25.75 ATOM 2240 CD1 ILE A 289 7.294 15.640 28.613 1.00 29.37 ATOM 2241 N THR A 290 8.811 19.790 27.210 1.00 22.42 ATOM 2243 C THR A 290 11.030 18.880 26.774 1.00 20.56 ATOM 2244 O THR A 290 11.030 18.880 26.774 1.00 20.56 ATOM 2245 CB THR A 290 11.301 18.880 26.774 1.00 20.56 ATOM 2247 OG1 THR A 290 11.243 18.743 27.986 1.00 19.81 ATOM 2247 OG1 THR A 290 11.301 18.800 26.774 1.00 20.56 ATOM 2247 OG1 THR A 290 11.301 18.800 26.774 1.00 20.56 ATOM 2247 OG1 THR A 290 11.301 18.800 26.774 1.00 20.56 ATOM 2247 OG1 THR A 290 10.823 21.761 27.308 1.00 21.70 ATOM 2247 OG1 THR A 290 11.301 18.800 26.774 1.00 20.15 ATOM 2248 N ILE A 291 11.757 18.296 25.841 1.00 19.36 ATOM 2250 C ILE A 291 11.757 18.296 25.841 1.00 19.36 ATOM 2251 O ILE A 291 11.464 17.865 25.286 1.00 19.73 ATOM 2251 O ILE A 291 11.467 15.609 27.044 1.00 20.06 ATOM 2252 CB ILE A 291 11.467 15.609 27.044 1.00 20.06 ATOM 2255 CG1 ILE A 291 11.467 15.609 27.044 1.00 20.06 ATOM 2255 CG1 ILE A 291 11.467 15.609 27.044 1.00 20.06 ATOM 2255 CG1 ILE A 291 11.467 15.609 27.044 1.00 20.06 ATOM 2256 N THR A 292 15.258 15.992 26.085 1.00 19.77 ATOM 2256 CG2 THR A 292 15.559 17.691 25.755 1.00 19.81 ATOM 2256 N THR A 292 15.559 17.691 25.755 1.00 19.81 ATOM 2250 CB THR A 292 15.559 17.691 25.755 1.00 19.81 ATOM 2256 N THR A 292 15.559 17.691 25.755 1.00 19.81 ATOM 2266 CB THR A 292 17.589 17.691 25.755 1.00 19.81 ATOM 2266 CB THR A 292 17.589 17.691 25.755 1.00 19.81 ATOM 2266 CB THR A 292 17.589 17.691 25.755 1.00 19.81 ATOM 2266 CB THR A 292 17.589 17.691 25.755 1.00 19.81 ATOM 2266 CB THR A 292 17.589 17.691 25.755 1.00 19.81 ATOM 2266 CB THR A 292 17.589 17.691 25.755 1.00 19.81 ATOM 2266 CB THR A 29				4.808			
ATOM 2233 N ILE A 289				5.548			
ATOM 2234 CA ILE A 289				5.220			
ATOM 2235 C ILE A 289 7.601 19.374 26.874 1.00 23.28 ATOM 2236 O ILE A 289 7.324 18.958 25.755 1.00 23.68 ATOM 2237 CB ILE A 289 6.750 18.123 28.817 1.00 24.68 ATOM 2238 CG1 ILE A 289 6.819 16.912 27.901 1.00 26.90 ATOM 2239 CG2 ILE A 289 5.648 17.983 29.885 1.00 25.75 ATOM 2240 CD1 ILE A 289 7.294 15.640 28.613 1.00 29.37 ATOM 2241 N THR A 290 8.811 19.790 27.210 1.00 22.42 ATOM 2242 CA THR A 290 9.904 19.768 26.264 1.00 21.38 ATOM 2243 C THR A 290 11.030 18.880 26.774 1.00 20.56 ATOM 2244 O THR A 290 11.243 18.743 27.986 1.00 19.81 ATOM 2245 CB THR A 290 10.461 21.175 26.053 1.00 21.70 ATOM 2246 OG1 THR A 290 9.405 22.108 25.460 1.00 20.15 ATOM 2248 N ILE A 291 11.757 18.296 25.841 1.00 19.36 ATOM 2249 CA ILE A 291 11.757 18.296 25.841 1.00 19.36 ATOM 2249 CA ILE A 291 12.903 17.503 26.190 1.00 19.73 ATOM 2250 C ILE A 291 13.862 17.976 24.083 1.00 20.08 ATOM 2251 O ILE A 291 13.862 17.976 24.083 1.00 20.08 ATOM 2253 CG1 ILE A 291 13.862 17.976 24.083 1.00 19.29 ATOM 2255 CB ILE A 291 13.862 17.976 24.083 1.00 19.29 ATOM 2250 C ILE A 291 13.862 17.976 24.083 1.00 20.08 ATOM 2250 C ILE A 291 13.862 17.976 24.083 1.00 19.29 ATOM 2250 C ILE A 291 13.862 17.976 24.083 1.00 19.81 ATOM 2250 C ILE A 291 13.862 17.976 24.083 1.00 19.29 ATOM 2250 C ILE A 291 13.873 15.214 26.378 1.00 20.08 ATOM 2250 C THR A 292 17.569 15.215 18.070 25.882 1.00 18.95 ATOM 2250 C THR A 292 17.589 17.691 25.753 1.00 19.17 ATOM 2250 C THR A 292 17.589 17.691 25.753 1.00 19.18 ATOM 2250 C THR A 292 17.589 17.691 25.753 1.00 19.18 ATOM 2250 C THR A 292 17.589 17.691 25.753 1.00 19.18 ATOM 2260 CB THR A 292 17.589 17.691 25.753 1.00 19.18 ATOM 2261 OG1 THR A 292 17.589 17.691 25.753 1.00 19.18 ATOM 2262 CG2 THR A 292 17.787 20.350 24.270 1.00 20.23 ATOM 2262 CG2 THR A 292 17.787 20.350 24.270 1.00 20.23 ATOM 2263 N VAL A 293 19.809 16.824 25.387 1.00 19.58 ATOM 2266 C VAL A 293 19.809 16.824 25.387 1.00 19.58 ATOM 2266 C VAL A 293 20.962 17.792 23.535 1.00 18.47 ATOM 2266 O VAL A 293 20.962 17.792 23.535 1.00 18.47 ATOM 2267 CB VAL A 293 20.9				6.571	19.406		
ATOM 2236 O ILE A 289				7.601	19.374		
ATOM 2237 CB ILE A 289 6.819 16.912 27.901 1.00 26.90 ATOM 2238 CG1 ILE A 289 5.648 17.983 29.885 1.00 25.75 ATOM 2240 CD1 ILE A 289 7.294 15.640 28.613 1.00 29.37 ATOM 2241 N THR A 290 8.811 19.790 27.210 1.00 22.42 ATOM 2242 CA THR A 290 9.904 19.768 26.264 1.00 21.38 ATOM 2243 C THR A 290 11.030 18.880 26.774 1.00 20.56 ATOM 2244 O THR A 290 11.030 18.880 26.774 1.00 20.56 ATOM 2245 CB THR A 290 10.461 21.175 26.053 1.00 19.81 ATOM 2246 OG1 THR A 290 10.823 21.761 27.308 1.00 20.15 ATOM 2248 N ILE A 291 11.757 18.296 25.841 1.00 19.36 ATOM 2249 CA ILE A 291 11.757 18.296 25.841 1.00 19.36 ATOM 2250 C ILE A 291 11.757 18.296 25.286 1.00 19.29 ATOM 2251 O ILE A 291 13.862 17.976 24.083 1.00 19.29 ATOM 2252 CB ILE A 291 13.862 17.976 24.083 1.00 19.29 ATOM 2253 CG1 ILE A 291 13.862 17.976 24.083 1.00 20.15 ATOM 2254 CG2 ILE A 291 13.873 15.214 26.378 1.00 20.21 ATOM 2255 CD ILE A 291 11.467 15.609 27.044 1.00 20.06 ATOM 2255 CD ILE A 291 13.873 15.214 26.378 1.00 20.21 ATOM 2255 CD ILE A 291 13.873 15.214 26.378 1.00 20.21 ATOM 2255 CD ILE A 291 13.873 15.214 26.378 1.00 20.21 ATOM 2255 CD ILE A 291 13.873 15.214 26.378 1.00 20.21 ATOM 2256 N THR A 292 17.589 17.691 25.753 1.00 19.17 ATOM 2258 C THR A 292 17.589 17.691 25.753 1.00 19.18 ATOM 2258 C THR A 292 17.589 17.691 25.753 1.00 19.18 ATOM 2258 C THR A 292 17.589 17.691 25.753 1.00 19.18 ATOM 2260 CB THR A 292 17.589 17.691 25.753 1.00 19.21 ATOM 2261 OG1 THR A 292 17.589 17.691 25.753 1.00 19.25 ATOM 2262 CG2 THR A 292 17.579 20.754 24.879 1.00 20.23 ATOM 2263 N VAL A 293 18.530 17.314 24.903 1.00 19.58 ATOM 2264 CA VAL A 293 18.530 17.314 24.903 1.00 19.58 ATOM 2266 O VAL A 293 20.962 17.792 23.535 1.00 19.58 ATOM 2266 O VAL A 293 20.962 17.792 23.535 1.00 19.58 ATOM 2266 O VAL A 293 20.962 17.792 23.535 1.00 19.58				7.324	18.958	25.755	
ATOM 2238 CG1 ILE A 289					18.123	28.817	
ATOM 2239 CG2 ILE A 289						27.901	
ATOM 2240 CD1 ILE A 289 7.294 15.640 28.613 1.00 29.37 ATOM 2241 N THR A 290 8.811 19.790 27.210 1.00 22.42 ATOM 2242 CA THR A 290 11.030 18.880 26.274 1.00 21.38 ATOM 2243 C THR A 290 11.030 18.880 26.774 1.00 20.56 ATOM 2244 O THR A 290 11.243 18.743 27.986 1.00 19.81 ATOM 2245 CB THR A 290 10.461 21.175 26.053 1.00 21.70 ATOM 2246 OG1 THR A 290 10.823 21.761 27.308 1.00 20.15 ATOM 2247 CG2 THR A 290 9.405 22.108 25.460 1.00 21.76 ATOM 2248 N ILE A 291 11.757 18.296 25.841 1.00 19.36 ATOM 2249 CA ILE A 291 12.903 17.503 26.190 1.00 19.36 ATOM 2250 C ILE A 291 12.903 17.503 26.190 1.00 19.29 ATOM 2251 O ILE A 291 13.862 17.976 24.083 1.00 19.29 ATOM 2252 CB ILE A 291 13.862 17.976 24.083 1.00 19.81 ATOM 2253 CG1 ILE A 291 13.862 17.976 24.083 1.00 20.08 ATOM 2253 CG1 ILE A 291 11.467 15.609 27.044 1.00 20.06 ATOM 2255 CD1 ILE A 291 13.873 15.214 26.378 1.00 21.77 ATOM 2256 N THR A 292 15.215 18.070 25.882 1.00 19.17 ATOM 2257 CA THR A 292 15.215 18.070 25.882 1.00 19.17 ATOM 2257 CA THR A 292 17.589 17.691 25.753 1.00 19.17 ATOM 2258 C THR A 292 17.589 17.691 25.753 1.00 19.18 ATOM 2250 CB THR A 292 17.589 17.691 25.753 1.00 19.18 ATOM 2260 CB THR A 292 17.589 17.691 25.753 1.00 19.18 ATOM 2261 OG1 THR A 292 17.787 20.350 24.270 1.00 20.23 ATOM 2261 OG1 THR A 292 17.787 20.350 24.270 1.00 20.23 ATOM 2262 CG2 THR A 292 17.787 20.350 24.270 1.00 20.23 ATOM 2263 N VAL A 293 19.809 16.824 25.387 1.00 19.58 ATOM 2266 CA VAL A 293 19.809 16.824 25.387 1.00 19.58 ATOM 2266 CA VAL A 293 19.809 16.824 25.387 1.00 19.58 ATOM 2266 CA VAL A 293 20.962 17.792 23.535 1.00 19.73 ATOM 2266 O VAL A 293 20.962 17.792 23.535 1.00 18.47 ATOM 2266 O VAL A 293 20.962 17.792 23.535 1.00 19.73 ATOM 2266 O VAL A 293 20.962 17.792 23.535 1.00 19.73 ATOM 2266 CB VAL A 293 20.962 17.792 23.535 1.00 19.73 ATOM 2266 O VAL A 293 20.962 17.792 23.535 1.00 19.73 ATOM 2266 O VAL A 293 20.962 17.792 23.535 1.00 19.73 ATOM 2266 O VAL A 293 20.962 17.792 23.535 1.00 19.73 ATOM 2266 O VAL A 293 20.962 17.792 23.535 1.00 19.73 ATOM 2267 CB VAL A 29						29.885	
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ATOM 2252 CB ILE A 291 12.598 15.992 26.085 1.00 20.08 ATOM 2253 CG1 ILE A 291 11.467 15.609 27.044 1.00 20.06 ATOM 2254 CG2 ILE A 291 13.873 15.214 26.378 1.00 20.21 ATOM 2255 CD1 ILE A 291 11.028 14.131 26.931 1.00 21.77 ATOM 2256 N THR A 292 15.215 18.070 25.882 1.00 18.95 ATOM 2257 CA THR A 292 16.406 18.407 25.156 1.00 19.17 ATOM 2258 C THR A 292 17.589 17.691 25.753 1.00 19.18 ATOM 2259 O THR A 292 17.671 17.497 26.965 1.00 19.21 ATOM 2260 CB THR A 292 16.703 19.937 25.259 1.00 19.83 ATOM 2261 OG1 THR A 292 15.559 20.724 24.879 1.00 20.23 ATOM 2262 CG2 THR A 292 17.787 20.350 24.270 1.00 20.15 ATOM 2263 N VAL A 293 18.530 17.314 24.903 1.00 19.25 ATOM 2265 C VAL A 293 19.809 16.824 25.387 1.00 19.51 ATOM 2266 O VAL A 293 20.912 17.667 24.749 1.00 19.58 ATOM 2266 O VAL A 293 20.912 17.667 24.749 1.00 19.58 ATOM 2266 CB VAL A 293 20.962 17.792 23.535 1.00 18.47 ATOM 2267 CB VAL A 293 20.962 17.792 23.535 1.00 19.73 ATOM 2267 CB VAL A 293 20.962 17.792 23.535 1.00 19.73 ATOM 2267 CB VAL A 293 20.962 17.792 23.535 1.00 19.73 ATOM 2267 CB VAL A 293 20.962 17.792 23.535 1.00 19.73 ATOM 2267 CB VAL A 293 20.962 17.792 23.535 1.00 19.73 ATOM 2267 CB VAL A 293 20.962 17.792 23.535 1.00 19.73 ATOM 2267 CB VAL A 293 20.962 17.792 23.535 1.00 19.73 ATOM 2267 CB VAL A 293 20.962 17.792 23.535 1.00 19.73							
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ATOM 2267 CB VAL A 233 21 400 14 951 25 250 1 00 20 24							
ATOM 2268 CG1 VAL A 293 21.490 14.951 25.250 1.00 20.24							
	MOTA	4 2268	CGI VAL A 293	∠1.49	O 14.33		

ATOM	2269	CG2					19.146	14.478	25.968		20.65		С
MOTA	2270		ASN				21.766	18.277	25.569		19.85		N
MOTA	2271		ASN				22.882	19.057	25.039		20.26		С
MOTA	2272	С	ASN				24.179	18.232	25.052		20.35		С
MOTA	2273	0	ASN				24.233	17.131	25.634		21.82		0
ATOM	2274	CB	ASN				23.008	20.443	25.727		20.82		С
MOTA	2275	CG	ASN				23.676	20.388	27.102		21.84		С
MOTA	2276	QD1					24.209	19.354	27.495		21.66		0
ATOM	2277	ND2					23.630	21.519	27.849		21.23		N
ATOM	2278	N	PHE				25.186	18.729	24.346		20.69		N
ATOM	2279	CA	PHE				26.490	18.095	24.233	•	20.46		C
MOTA	2280	С			295		27.452	19.240	24.494		21.42		C
ATOM	2281	0			295		27.573	20.167	23.653		20.85		0 C
ATOM	2282	CB			295		26.728	17.569	22.814		20.62		
MOTA	2283	CG			295		25.898	16.366	22.440		21.15		C
ATOM	2284		PHE				24.526	16.468	22.247		21.98		C
ATOM	2285		PHE				26.498	15.130	22.256		19.31	•	C
ATOM	2286		PHE				23.791	15.343	21.902		19.77		C
ATOM	2287		PHE				25.762	14.037	21.885		17.96 17.87		C
MOTA	2288 2289	N ·			295 296		24.424 28.123	14.138 19.196	21.720 25.645		21.19		И
ATOM ATOM	2290	CA			296		29.023	20.275	26.050		21.19	•	C
ATOM	2291	CA			296		30.481	19.834	25.873		21.40		C
ATOM	2292	Ö			296		30.898	18.795	26.387		21.96		Õ
MOTA	2293	СВ			296		28.760	20.669	27.498		21.13		C
ATOM	2294	CG			296		27.853	21.859	27.710		21.95		Č
ATOM	2295	CD1			296		27.797	22.987	26.955		23.23		Ċ
MOTA	2296	CD2			296		26.935	22.067	28.797		22.27		Ċ
MOTA	2297	NE1			296		26.882	23.869	27.478		22.26		N
MOTA	2298	CE2	TRP	Α	296		26.336	23.329	28.607	1.00	22.53		С
MOTA	2299	CE3	TRP	Α	296		26.531	21.298	29.894	1.00	24.83		С
MOTA	2300	CZ2	TRP	Α	296		25.362	23.840	29.463	1.00	22.34		С
MOTA	2301	CZ3	TRP	Ά	296		25.557	21.810	30.754	1.00	24.59	•	С
MOTA	2302	CH2			296		24.993	23.075	30.531		23.75		С
MOTA	2303	N			297		31.235	20.632	25.126		21.64		N
ATOM	2304	CA			297		32.633	20.361	24.845		21.81	•	C
ATOM	2305	С			297		33.482	21.523	25.320		22.41		C
ATOM	2306	0			297		33.110	22.682	25.146		21.78		0
MOTA	2307	CB			297		32.862	20.198	23.344		21.49		C
ATOM ATOM	2308 2309	CG.			297 297		32.287	18.943	22.761 22.415		21.77		C
ATOM	2310				297		30.934	18.870			21.68		C
ATOM	2311				297		33.083	17.841 17.734	22.526 21.890		19.80 22.16		c
ATOM	2312				297		32.555	16.690	21.993		20.99		c
ATOM	2313	CZ			297		31.215	16.637	21.686		21.46		Ċ
ATOM	2314	ОН			297		30.673	15.494	21.159		22.11		ō
ATOM	2315	N			298		34.632	21.220	25.899		23.17		N
MOTA	2316	CA			298		35.566	22.273	26.288		24.45		С
MOTA	2317	С			298		36.074	22.912	25.021		24.21		. C
MOTA	2318	0			298		36.264	22.228	24.025		23.35		0
MOTA	2319	CB	LYS	S A	298		.36.748	21.699	27.085	1.00	24.85		С
MOTA	2320	CG	LYS	A	298		36.436	21.416	28.552	1.00	28.00		C
MOTA	2321				298		37.657	20.865	29.298		31.59		C
MOTA	2322	CE			298		37.309	20.447	30.730		33.77		С
MOTA	2323	NZ			298		38.406	19.627	31.367		36.02		N
MOTA	2324	N			299		36.317	24.216	25.056		25.28		N
MOTA	2325	CA			299		36.818	24.909	23.886		26.38		C
ATOM	2326	C			299		38.254	24.542	23.547		27.78		C
ATOM	2327	0			299		38.935	23.895	24.315		27.16		0
ATOM	2328	N			300	•	38.690	24.949	22.366		30.42		N C
MOTA	2329	CA	ΑLL	1 A	300		40.062	24.762	21.918	1.00	32.93		C

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	ATOM	2330	С	ALA A	300		41.021	25.544	22.819	1.00 3			С
	ATOM	2331	0	ALA A	300		40.597	26.337	23.646	1.00 3	4.87		0
	ATOM	2332			300 A		40.199	25.249	20.472	1.00 3	2.98		С
					A 301		42.318	25.355	22.615	1.00 3			N
	MOTA	2333						26.012	23.440	1.00 4			C
	MOTA	2334	CA		A 301		43.347						c
	ATOM	2335	С		A·301		43.548	27.484	23.102	1.00 4			
	MOTA	2336	0	PRO A	A 301		43.379	27.853	21.950	1.00 4			0
	MOTA	2337	CB	PRO Z	A 301		44.615	25.246	23.061	1.00 4	10.42		С
	ATOM	2338	CG		A 301		44.397	24.879	21.638	1.00 3	39.87		С
	ATOM	2339	CD		A 301		42.919	24.544	21.535	1.00 3	38.98		C
			N		A 302		43.915	28.293	24.090	1.00 4			N
	MOTA	2340						29.725	23.912	1.00			C
	MOTA	2341	CA		A 302		44.209			1.00			Č
	MOTA	2342	С		A 302		45.593	29.790	23.315				
	ATOM	2343	0	THR .	A 302		46.534	29.388	23.992	1.00			0
	MOTA	2344	CB	THR	A 302		44.242	30.391	25.294	1.00	46.57		С
	MOTA	2345	OG1	THR	A 302		42.941	30.320	25.895	1.00	48.00		0
	ATOM	2346	CG2		A 302		44.526	31.869	25.199	1.00	47.24		С
		2347	N		A 303		45.782	30.336	22.112	1.00	48.55		N
	MOTA				A 303		47.090	30.170	21.473	1.00			С
	MOTA	2348	CA						22.341	1.00			C
	MOTA	2349	С		A 303		48.210	30.717				•	ő
	ATOM	2350	0		A 303		47.874	31.450	23.269	1.00			
	MOTA	2351	CB	PRO	A 303		46.967	30.980	20.185	1.00			C
•	MOTA ·	2352	CG	PRO	A 303		45.504	31.101	19.952	1.00			С
	MOTA	2353	CD	PRO	A 303		44.916	31.243	21.330	1.00	48.62		С
	MOTA	2354	N		A 307		46.795	36.776	18.436	1.00	52.62		И.
		2355	CA		A 307		46.885	37.814	17.415	1.00	52.76		С
	ATOM						45.865	38.906	17.636		52.00		С
	MOTA	2356	C		A 307				18.096		52.48		· 0
	MOTA	2357	0		A 307		44.757	38.658					Ċ
	MOTA	2358	CB		A 307		_. 46.686	37.246	15.996		53.32		
	MOTA	2359	CG	${ t GLU}$	A 307		46.893	38.307	14.908		54.63		C
	ATOM	2360	CD	GLU	A 307		46.862	37.764	13.487		56.43		C
	MOTA	2361		GLU	A 307		46.527	36.574	13.290	1.00	57.49		0
	ATOM	2362			A 307		47.173	38.543	12.558	1.00	57.89		0
	ATOM	2363	N		A 308		46.255	40.125	17.303		51.19		N
							45.367	41.267	17.405		50.55		С
	MOTA	2364	CA		A 308				16.039		49.51		Ċ
	MOTA	2365	С		A 308		44.747	41.494				•	ŏ
	MOTA	2366	0		A 308		45.300	41.053	15.028		49.70		
	MOTA	2367	CB	TYR	A 308		46.151	42.485			50.82		C
	MOTA	2368	CG	TYR	A 308		46.702	42.286	19.259		52.47		С
	ATOM ·	2369	CDI	LTYR	A 308		45.949	42.632	20.373	1.00	53.15		С
	MOTA	2370			A 308		47.948	41.696	19.462	1.00	53.79		C
	ATOM	2371			A 308		46.426			1.00	54.22		С
				D WAD	A 308	,	48.437				54.76		С
	ATOM	2372					47.670				55.10		С
	ATOM	2373			A 308						56.68		ō
	ATOM	2374			A 308		48.146						Ŋ
	MOTA	2375			A 309		43.584				47.88	•	
	MOTA	2376	CA	PRO	A 30	€	42.843				46.21		C
	MOTA	2377	C	PRO	A 30	•	42.139	41.503	17.952	1.00	43.75		С
	MOTA	2378		PRO	A 30	3 ·	41.768	40.503	17.369	1.00	44.10		0
	ATOM	2379			A 30		41.804		16.562	1.00	46.39		С
		2380			A 30		41.610			. 1.00			С
	ATOM						42.899				48.06		С
	ATOM	2381			A 30						40.94		N
	MOTA	2382			A 31		41.973						C
	MOTA	2383			J A 31		41.349				38.75		
	MOTA	2384	l C	LEU	J A 31	0	39.863				36.87		C
	MOTA	2385		LEU	J A 31	0	39.148	41.474			37.02		0
	MOTA	2386			J A 31		41.499	41.017	21.566		38.63		С
	MOTA	2387			A 31		42.571			1.00	37.97		С
	ATOM	2388			A 31		43.840				37.27		С
					J A 31		42.836				37.27		С
	MOTA	2389					39.392				34.04		N
	ATOM	2390	ИС	ĿΫ́	5 A 31	4	33.334	. 59.254	, 19.04		. 51.01		

ATOM	2391	CA :	LYS A 311	37.972	38.998	19.702	1.00 32.20		С
MOTA	2392	C	LYS A 311	37.208	39.376	20.968	1.00 30.33		С
ATOM	2393	0	LYS A 311	37.760	39.421	22.072	1.00 29.17		0
ATOM	2394		LYS A 311	37.733	37.564	19.371	1.00 32.59		C
MOTA	2395		ALA A 312	35.924	39.641	20.788	1.00 28.23		N
MOTA	2396		ALA A·312	35.074	40.011	21.895	1.00 27.38		С
MOTA	2397		ALA A 312	35.148	38.973	23.005	1.00 26.28		C
MOTA	2398		ALA A 312		39.334	24.172	1.00 24.54		0
MOTA	2399		ALA A 312		40.205	21.421	1.00 27.09		C N
ATOM	2400		HIS A 313		37.689	22.649	1.00 25.72		C
MOTA	2401		HIS A 313		36.669 36.609	23.674 24.428	1.00 25.82 1.00 24.79		C
ATOM	2402		HIS A 313		36.183	25.557	1.00 24.79	•	Ö
MOTA	2403 2404		HIS A 313		35.293	23.129	1.00 24.13		Č
ATOM ATOM	2404	CG	HIS A 313		34.641	22.303	1:00 29.84		Č
ATOM	2405		HIS A 313		34.903	20.954	1.00 35.52		N
ATOM	2407		HIS A 313		33.746	22.627	1.00 33.54		C
ATOM	2408		HIS A 313		34.208	20.489	1.00 35.03		С
ATOM	2409		HIS A 313		33.491	21.481	1.00 35.78		N
ATOM	2410	N	GLN A 314		37.042	23.803	1.00 24.43		N
MOTA	2411	CA	GLN A 314	38.762	37.092	24.465	1.00 24.34		, C
ATOM	2412	С	GLN A 314	38.762	38.226	25.510	1.00 24.39		С
MOTA	2413	0	GLN A 314		38.081	26.590	1.00 24.82		0
MOTA	2414	CB	GLN A 314		37.290	23.439	1.00 24.47		C
ATOM	2415	CG	GLN A 314		36.106	22.472	1.00 25.49		C
MOTA	2416	CD	GLN A 314		36.362	21.366	1.00 25.52		. c
MOTA	2417		GLN A 314		37.287	20.563	1.00 27.59		N
ATOM	2418		GLN A 314		35.553	21.330	1.00 28.22 1.00 23.51		N
ATOM	2419	N	LYS A 31!		39.337 40.423	25.196 26.154	1.00 23.31		C
ATOM	2420	CA	LYS A 31			27.325	1.00 23.73		c
MOTA	2421 2422	C	LYS A 315			28.465	1.00 21.38		ŏ
MOTA MOTA	2422	СВ	LYS A 31			25.504	1.00 24.09		č
MOTA	2424	CG	LYS A 31			24.533	1.00 26.96		C
ATOM	2425	CD	LYS A 31			23.947	1.00 31.28		С
ATOM	2426	CE	LYS A 31			22.977	1.00 34.34		С
ATOM	2427	NZ	LYS A 31			22.005	1.00 36.25		- N
ATOM	2428	N	VAL A 31	6 36,109	39.177	27.041	1.00 22.30		N
MOTA	2429	CA	VAL A 31	6 35.276		28.113	1.00 22.39		С
MOTA	2430	С	VAL A 31			29.063	1.00 22.29		С
MOTA	2431	0	VAL A 31			30.274	1.00 21.27		0
MOTA	2432		VAL A 31						C
MOTA	2433		VAL A 31			28.750			C
MOTA	2434		VAL A 31			26.802 28.499			N
MOTA	2435	N CA	ALA A 31 ALA A 31			29.295			C
ATOM ATOM	2436 2437	CA	ALA A 31			30.164			C
ATOM	2437	Ö	ALA A 31			31.300		•	o
ATOM	2439		ALA A 31			28.380			С
ATOM	2440	N	ILE A 31			29.606			N
ATOM	2441		ILE A 31			30.318			С
ATOM	2442		ILE A 31			31.524			С
MOTA	2443		ILE A 31			32.646	1.00 20.76		0
ATOM	2444		ILE A 31	8 40.709	40.023	29.377	1.00 20.58		С
MOTA	2445		L ILE A 31						C
MOTA	2446		2 ILE A 31						C
ATOM	2447		L ILE A 31						C
ATOM	2448		MET A 31						N
ATOM	2449		MET A 31						C
ATOM	2450		MET A 31						C
MOTA	2451	. 0	MET A 31	.9 37.32	6 39.911	34.651	. 1.00 21.13		0

ATOM	2452		MET A		36.17		31.818	1.00 21.01	C
ATOM	2453		MET A		36.42		30.971	1.00 21.17	C
MOTA	2454		MET A		34.86		30.459	1.00 22.71	S
MOTA	2455	CE	MET A		34.20		29.206	1.00 22.13	C
MOTA	2456	N	ARG A		36.76		33.068	1.00 21.34	Ŋ
ATOM	2457	CA	ARG A		36.53		34.075	1.00 21.12	C
MOTA	2458	С	ARG A		37.80		34.898	1.00 21.25	С
ATOM	2459	0	ARG A	320	37.74	7 37.064	36.122	1.00 21.48	0
MOTA	2460	CB	ARG A	320	36.10	2 36.095	33.427	1.00 21.01	С
MOTA	2461	CG	ARG A	320	34.72		32.741	1.00 20.63	С
MOTA	2462	CD	ARG A	320	34.32	4 34.795	32.142	1.00 18.73	C
ATOM	2463	NE	ARG A	320	34.22	5 33.824	33.225	1.00 19.25	N
ATOM	2464	CZ	ARG A	320	33.24	7 33.809	34.115	1.00 19.86	, C
ATOM	2465	NH1	ARG A	320	32.25	9 34.689	34.062	1.00 21.08	· N
ATOM	2466		ARG A		33.26	32.923	35.081	1.00 23.29	N
ATOM	2467	N	ASN A		38.94		34.231	1.00 20.94	N
ATOM	2468	CA	ASN A		40.18		34.939	1.00 20.88	С
MOTA	2469	С	ASN F		40.53		35.916	1.00 20.93	С
ATOM	2470	0	ASN A		40.96		37.047	1.00 21.77	0
ATOM	2471	СВ	ASN A		41.32		33.958	1.00 21.04	С
ATOM	2472	CG	ASN A		41.28		33.447	1.00 22.80	С
ATOM	2473		ASN A		40.92		34.185	1.00 23.97	0
ATOM	.2474		ASN A		41.66		32.193	1.00 21.35	N
MOTA	2475	N		A 322	40.35		35.505	1.00 20.14	N
ATOM	2476	CA		A 322	40.63		36.408	1.00 20.06	С
MOTA	2477	C		A 322	39.7		37.650	1.00 19.42	С
ATOM .	2478	Ö		A 322	40.20		38.767	1.00 18.73	
ATOM	2479	СВ		A 322	40.3		35.715	1.00 20.21	C
ATOM	2480	CG1		A 322	41.3		34.535	1.00 21.54	C
ATOM	2481		ILE A		40.5			1.00 20.53	C
	2482		ILE		42.8		34.868	1.00 24.56	Ċ
ATOM		N		A 323	38.4	•	37.454	1.00 18.94	Ŋ
MOTA	2483				37.5			1.00 18.98	C
MOTA	2484	CA		A 323				1.00 19.33	Č
ATOM	2485	C		A 323	38.0			1.00 19.05	ő
ATOM	2486	0		A 323 A 323	38.0 36.1			1.00 19.05	. C
MOTA	2487	CB						1.00 19.34	C
ATOM	2488	CG		A 323	35.5			1.00 13.34	C
ATOM	2489	CD		A 323	34.1			1.00 19.19	ő
MOTA	2490	OEI		A 323	33.1			1.00 19.15	. 0
MOTA	2491		GLU .		34.0			1.00 19.55	. O
ATOM	2492	N		A 324	38.4				Č
MOTA	2493	CA		A 324	38.8			1.00 20.24 1.00 20.68	c
MOTA	2494	С		A 324	40.1			1.00 20.83	o
ATOM	2495	0		A 324	40.1				C
MOTA	2496	CB		A 324	39.1			1.00 20.07	C
ATOM	2497	CG		A 324	37.9				.c
MOTA	2498	CD		A 324	38.3				0
ATOM	2499	CE		A 324	37.1				C
MOTA	2500	NZ		A 324	37.5				N
MOTA	2501			A 325	41.1				N
MOTA	2502			A 325	42.3				C
MOTA	2503			A 325	42.1				C
MOTA	2504			A 325	42.7				0
MOTA	2505			A 325	43.3				
MOTA	2506	CG		A 325	43.9				
MOTA	2507	SD		A 325	44.7				
MOTA	2508	CE		A 325	45.6				
ATOM	2509		LEU	A 326	41.3				
MOTA	2510			A 326	41.0				
MOTA	2511	. С	LEU	A 326	40.3				
MOTA	2512		LEU	A 326	40.7	735 40.41	7 44.795	1.00 22.40	0

ATOM	2513	CB	LEU A	326	4 (0.151	41.735	41.865	1.00 2			С
ATOM	2514	CG	LEU A	326	4 (0.677	43.139	41.625	1.00 2	25.86	•	С
ATOM	2515	CD1	LEU A	326	4:	2.187	43.277	41.529	1.00 2	26.53		С
ATOM	2516		LEU A		3	9.986	43.672	40.377	1.00 2	25.54		С
ATOM	2517		GLY A			9.441	39.164	43.460	1.00 2	23.29		N
MOTA	2518		GLY A			8.760	38.489	44.547	1.00 2			С
	2519		GLY P			9.728	37.723	45.418	1.00 2			С
MOTA			GLY F			9.659	37.783	46.649	1.00 2			0
ATOM ·	2520					0.644	37.703	44.778	1.00 2			N
ATOM	2521		GLU F				36.265	45.506	1.00 2			C
ATOM	2522		GLU A			1.671						c
ATOM	2523	С	GLU A			2.661	37.180		1.00			0
ATOM	2524	0	GLU A			3.029	36.926		1.00			
MOTA	2525	CB	GLU A			2.442	35.368	44.546	1.00			C
MOTA	2526	CG	GLU A			1.576	34.278	43.947	1.00			C
ATOM	2527	CD	GLU A	A 328		1.719 [.]			1.00			C
ATOM	2528		GLU A			2.091	32.986		1.00			0
MOTA	2529	OE2	GLU Z	A 328		1.483	31.896	44.034	1.00			0
ATOM	2530	N		A 329	· 4	3.094	38.240	45.552	1.00	24.91		N
ATOM	2531	CA		A 329		4.102	39.119	46.134	1.00	24.95		C
ATOM	2532	С	ALA Z	A 329	4	3.535	39.929	47.285	1.00	24.94		С
ATOM	2533	Ö	AT.A	A 329	4	4.197	40.147	48.276		24.57		0
MOTA	2534	СВ		A 329			40.022	45.088		24.88		С
ATOM	2535	N		A 330		2.290	40.354	47.161		25.47		N
	2536	CA		A 330 .		1.672	41.133	48.219		26.16		C
ATOM				A 330		1.212	40.265	49.379		26.80		Ċ
MOTA	2537	C						50.471		27.00		Õ
MOTA	2538	0		A 330		0.994				26.08		c
MOTA	2539	CB		A 330		10.504	41.930	47.669			•	C
MOTA	254.0	CG		A 330		10.954	42.981	46.653		26.04		C
MOTA	2541			A 330		39.760	43.489			26.16		
ATOM	2542	CD2		A 330		11.688				26.65		C.
ATOM	2543	N	GLY	A 331	4	11.037		49.126		27.87		N
MOTA	2544	CA	GLY	A 331	4	10.645	38.039	50.158		28.89		С
ATOM	2545	C.	GLY	A 331	:	39.176	38.086	50.526		29.43		С
ATOM	2546	0	GLY	A 331	;	38.763	37.435	51.478	1.00	30.62		0
MOTA	2547	N		A 332		38.400	38.887	49.808	1.00	.29.59		N
ATOM	2548	CA		A 332		36.963	38.995	50.023	1.00	29.64		С
ATOM	2549	С		A 332		36.367		48.718	1.00	29.00		С
ATOM	2550	ō		A 332		36.649			1:00	28.70	•	0
MOTA	2551	СВ		A 332		36.656				30.15		С
ATOM	2552	CG		A 332		35.162				31.82		С
ATOM	2553			A 332		34.335				34.71		0
ATOM				A 332			40.818			35.11		N
				A 333		35.528				28.53		Ŋ
ATOM	2555									28.25		Ċ
ATOM	2556			A 333		35.001				27.91		C
ATOM	2557			A 333		34.176				26.99		Ö
MOTA	2558			A 333		34.033						
MOTA	2559			A 333		34.120				28.16		C
ATOM	2560			A 333.		34.137				28.91	•	С
MOTA	2561			A 333		35.022				28.96		С
MOTA	2562	N		A 334		33.638				27.80		N
MOTA	2563	CA		A 334		32.814				27.97		C
MOTA	2564	С	GLN	A 334		33.665				26.77		С
MOTA	2565		GLN	A 334		33.144	44.245			26.51		0
ATOM	2566			A 334		31.906	41.867	49.278		28.98		С
ATOM	2567			A 334		30.675		49.038	1.00	32.17		С
MOTA	2568			A 334		29.661				35.54	•	С
ATOM	2569			A 334		29.682				37.92		0
ATOM	2570			A 334		28.760				36.72		N
ATOM	2571			A 335		34.974				25.19		N
ATOM	2572			A 335		35.860				24.41		C
	2572			A 335		36.170				22.68		Č
MOTA	2573	, .	GHO	r 222		50.170			2.00			-

ATOM	2574	0	GLU A 335	36.700	45.521	46.228	1.00 21.42	0
MOTA	2575		GLU A 335	37.150	43.928	48.835	1.00 24.98	C
MOTA	2576		GLU A 335	36.974	44.148	50.343	1.00 27.94	C
MOTA	2577	CD	GLU A 335	38.264	44.055	51.139	1.00 31.85 1.00 34.79	C 0
MOTA	2578		GLU A 335	39.248	44.736 43.312	50.777 52.158	1.00 34.79	0
ATOM	2579		GLU A. 335	38.298 35.809	43.512	45.625	1.00 30.87	N
MOTA	2580 2581	N CA	VAL A 336 VAL A 336	36.113	43.751	44.201	1.00 20.37	c
MOTA MOTA	2582	CA	VAL A 336	35.541	45.034	43.603	1.00 20.01	· c
ATOM	2583	0	VAL A 336	36.247	45.798	42.954	1.00 19.07	ō
MOTA	2584	CB.	VAL A 336	35.647	42.554	43.371	1.00 20.60	С
ATOM	2585	CG1		35.785	42.841	41.883	1.00 21.06	С
ATOM	2586		VAL A 336	36.463	41.316	43.743	1.00 20.68	С
ATOM	2587	N	GLY A 337	34.260	45.275	43.842	1.00 19.61	N
ATOM	2588	CA	GLY A 337	33.593	46.437	43.317	1.00 19.45	С
ATOM	2589	С	GLY A 337	34.205	47.760	43.731	1.00 19.51	C
MOTA	2590	0	GLY A 337	34.522	48.576	42.871	1.00 18.93	0
MOTA	2591	N	PRO A 338	34.333	48.010	45.032·	1.00 20.41	N
MOTA	2592	CA	PRO A 338	34.959		45.503	1.00 20.40	C
MOTA	2593	C	PRO A 338	36.368	49.500	44.923	1.00 20.13 1.00 19.20	0
ATOM	2594	0	PRO A 338	36.674	50.630	44.548 47.035	1.00 19.20	C
MOTA	2595	CB	PRO A 338			47.033	1.00 20.03	Ċ
ATOM ATOM	2596 2597	CG CD	PRO A 338			46.151	1.00 20.95	č
ATOM	2598	N	LEU A 339			44.831	1.00 20.34	Ŋ
ATOM	2599	CA	LEU A 339			44.234	1.00 20.55	С
ATOM	2600	C	LEU A 339			42.768	1.00 20.06	С
ATOM	2601	Ō	LEU A 339			42.330	1.00 19.61	0
ATOM	2602	СВ	LEU A 339		47.408	44.358	1.00 20.81	С
MOTA	2603	CG	LEU A 339	40.855	47.618	43.943	1.00 22.54	С
ATOM	2604	CD1				44.786	1.00 25.30	C
MOTA	2605	CD2	LEU A 339			42.496	1.00 23.17	C
MOTA	2606	N	LEU A 340			42.023	1.00 19.51	И
MOTA	2607	CA	LEU A 340			40.600	1.00 19.36	C
MOTA	2608	.C	LEU A 340			40.427 39.566	1.00 19.30 1.00 17.55	0
MOTA	2609	O	LEU A 340		L · 47.721	39.952	1.00 17.33	Č
ATOM ATOM	2610 2611	CB CG	LEU A 340			39.637	1.00 21.99	C
ATOM	2612		LEU A 340			39.069	1.00 22.03	C
ATOM	2613		LEU A 34			38.673	1.00 21.20	С
ATOM	2614	N	ASN A 34			41.270	1.00 19.17	N
ATOM	2615	CA	ASN A 34			41.232	1.00 20.20	С
MOTA	2616	С	ASN A 34				1.00 19.98	С
MOTA	2617	0	ASN A 34			40.848	1.00 19.61	0
MOTA	2618	CB	ASN A 34			42.196	1.00 20.66	С
MOTA	2619	CG	ASN A 34			41.619	1.00 24.17	C
MOTA	2620		L ASN A 34			40.531	1.00 30.93	О N
ATOM	2621		2 ASN A 34			42.317 42.558	1.00 26.37 1.00 20.07	N
MOTA	2622		THR A 34			42.556		C
MOTA	· 2623 2624		THR A 34			42.939		Ċ
MOTA MOTA	2625		THR A 34			41.502		Ō
ATOM	2626					44.189		, с
MOTA	2627					45.320		0
ATOM	2628		2 THR A 34					C
MOTA	2629		MET A 34				1.00 20.30	N
ATOM	2630			3 40.40	2 52.543			C
MOTA	2631	C	MET A 34				·	C
MOTA	2632		MET A 34					0
MOTA	2633							C
ATOM	2634	CG	MET A 34	3 41.81	0 50.453	39.625	1.00 23.39	С

ATOM	2635	SD	MET :	A	343	42.247	7 49.059	38.524	1.00 25.	69		s
ATOM	2636	CE	MET .			41.16		38.968	1.00 26.	74		С
ATOM	2637	N	ILE .	Α	344	38.633			1.00 20.	76		N
MOTA	2638	CA	ILE .	A	344	38.16			1.00 21.	23		C
MOTA	2639	С	ILE			37.648			1.00 20.			С
MOTA	2640	0	ILE			37.76			1.00 20.		,	0
MOTA	2641	CB	ILE			37.10			1.00 22.			С
MOTA	2642					35.71			1.00 23.			С
MOTA	2643		ILE			37.48			1.00 24.			С
ATOM	2644		ILE			34.65			1.00 28.			С
ATOM	2645	И	LYS			37.06			1.00 20.			N
ATOM	2646	CA	LYS			36.48			1.00 21.			C
ATOM	2647	C	LYS			37.46			1.00 19.			C
ATOM	2648	0	LYS			38.45			1.00 19	_		0 C
MOTA	2649	CB	LYS LYS			35.43			1.00 22			C
ATOM ATOM	2650 2651	CG CD	LYS			35.56 34.21			1.00 27			C
ATOM	2652	CE	LYS			33.39			1.00 30			C
ATOM	2653	NZ	LYS			34.06			1.00 37			N
ATOM	2654	N	GLY			37.14			1.00 18			N
MOTA	2655	CA	GLY			37.14			1.00 17			C
ATOM	2656	C	GLY			39.30			1.00 16			c
ATOM	2657	ŏ	GLY			40.17			1.00 16			ō
ATOM	2658	N	ARG			39.45				.85		N
ATOM	2659	CA	ARG			40.69			1.00 17			C
ATOM	2660	С	ARG			40.46				.57		С
ATOM	2661	0	ARG	Α	347	41.17			1.00 17	.10		0
ATOM	2662	CB	ARG	Α	347	41.37	9 57.38	4 36.812	1.00 17	.20		C
MOTA	2663	CG	ARG	A	347	41.82	2 57.94	38.181	1.00 16	.77 .		C
MOTA	2664	CD	ARG	A	347	43.28	7 57.49	1 38.583	1.00 18	.88		C
ATOM	2665	NE	ARG	Α	347	43.25	4 56.08	7 38.618	1.00 17	.77		N
MOTA	2666	CZ	ARG	A	347	44.11	5 55.22	38.149	1.00 16	.11		С
MOTA	2667		ARG			45.32	3 55.51	2 37.658	1.00 16	.59		N
MOTA	2668		ARG			43.73			1.00 13			N
MOTA	2669	N	TYR			39.47				.74		N
MOTA	2670	CA	TYR			39.13			1.00 20		•	С
MOTA	2671	С			348	37.67			1.00 21			C
ATOM	2672	0			348	37.29			1.00 22			0
ATOM	2673	CB	TYR			39.41			1.00 19			C
MOTA	2674	CG			348	40.87		•		. 65		C
ATOM	2675	CD1				41.66			1.00 18			C
MOTA	2676		TYR			41.45			1.00 17			C
ATOM	2677		TYR TYR			42.98			1.00 19			C
MOTA MOTA	2678 2679	CEZ			348	42.77 43.54			1.00 18 1.00 18			C
ATOM	2680	OH			348	44.85			1.00 18			C 0
ATOM	2681	N			349	36.83			1.00 17			N
ATOM	2682	CA			349	35.42						C
ATOM	2683	C			349	34.94			1.00 27			
ATOM	2684	Ö			349	35.64			1.00 28		•	Ċ
ATOM	2685	СВ			349	34.49						c
ATOM	2686	CG			349	34.51						c
ATOM ·	2687		ASN			35.28						ō
ATOM		· ND2				33.65					•	N
ATOM	2689		ASN			33.76			1.00 31			o
TER	2690				349	30.7		555				-
ATOM	2691	N			795	45.83	37 35.55	5 30.600	1.00 35	.49		N
ATOM	2692	CA			795	44.75					•	C
ATOM	2693	C			795	43.58						C
ATOM	2694	0			795	42.4						ō
ATOM	2695	CB			795	45.25						С
	_				_					_		

•												
MOTA	2696		LEU S			44.695	38.978	31.791	1.00			C
MOTA	2697		LEU S			44.761	38.459	33.204		37.65		C.
MOTA	2698		LEU S			45.450	40.289	31.718	1.00			
MOTA	2699		THR S			43.936	35.940	28.796		35.47		N C
ATOM	2700		THR S			43.060	35.351	27.800		36.25		
MOTA	2701		THR S			42.644	33.888	28.079		35.84		C
MOTA	2702	0	THR S			41.819	33.331	27.365		36.38		0
MOTA	2703		THR S			43.817	35.429	26.457		36.63		C
ATOM	2704		THR S			43.251	34.528	25.524		38.48		0
MOTA	2705		THR S			45.257	34.907	26.593		37.07		
ATOM	2706	N	SER S			43.197	33.251	29.101		35.44		N C
MOTA	2707	CA	SER S			42.835	31.860	29.377		35.29		C
MOTA	2708	С	SER S			41.426	31.760	29.984		35.18		. 0
MOTA	2709	0	SER S			40.925	32.701	30.611		33.96		
MOTA	2710	CB	SER S			43.856	31.189	30.291		35.17		C
MOTA	2711	OG	SER S		•	43.716	31.654	31.624		36.65		0
ATOM	2712	N	TYR S			40.789	30.611	29.790		35.36		N
MOTA	2713	ĊA	TYR S			39.427	30.430	30.256		35.94	•	C
MOTA	2714	С	TYR S			39.148	29.075	30.890		35.14		C
MOTA	2715	Ο.	TYR :			39.845	28.095	30.657		35.54		0
MOTA	2716	CB	TYR :			38.440	30.707	29.120		36.37		С
MOTA	2717	CG	TYR :			38.554	29.794	27.920		39.89		C
ATOM	2718	CD1				39.587	29.934	26.996		42.41		С
MOTA	2719	CD2				37.606	28.808	27.697		43.13		C
MOTA	2720	CE1				39.681	29.095	25.893		43.97		C
MOTA	2721	CE2				37.687	27.963	26.597		44.94		C
MOTA	2722	CZ	TYR			38.723	28.109	25.698		44.95		
MOTA	2723	OH	TYR			38.781	27.270	24.613		44.37		0
MOTA	2724	N	ASP			38.108	29.046	31.709		34.54		N
MOTA	2725	CA	ASP			37.685	27.840	32.392		33.87		C
MOTA	2726	C	ASP			36.600	27.187	31.545		32.58		C
MOTA	2727	0	ASP			36.465	27.501	30.366		32.32		O C
ATOM	2728	CB	ASP			37.140	28.208	33.770		34.50		C
MOTA	2729	CG	ASP			37.299	27.104	34.773		36.07		0
MOTA	2730			S 799		36.790	25.986	34.551		37.15		0
MOTA	2731			S 799		37.918	27.279	35.833		41.54		N
MOTA	2732	N		S 800		35.812	26.301	32.141		30.83		C
MOTA	2733	CA		S 800		34.798	25.586	31.392	1.00	29.83		c
MOTA	2734	C		S 800		33.490	25.511	32.161		28.68		o
MOTA	2735	0		s 800		32.794	24.502	32.092				C
MOTA	2736		CYS			35.273	24.167	31.092		29.46		S
ATOM	2737	SG		S 800		35.576	23.194	32.601		28.36		И
ATOM	2738			S 801		33.152	26.578	32.874		28.63		C
ATOM	2739			S 801		31.936	26.605			28.34		č
ATOM	2740			S 801		30.667	26.793			27.30		ő
ATOM	2741			S 801		30.626		31.867 34.751		28.61		Č
MOTA	2742			S 801		32.038	27.688			30.83		č
ATOM	2743			S 801		33.252	27.501 28.346			32.58		č
MOTA	2744			S 801		33.188	27.985			33.57	,	Õ
ATOM	2745			S 801		32.414				33.97		Ö
ATOM	2746			S 801		33.910				28.85		N
MOTA	2747			S 802		29.627				29.03		C
ATOM	2748			S 802		28.350				29.80		C
ATOM	2749			S 802		27.233						0
ATOM	2750			S 802		27.505				0 29.92 0 28.44		C
ATOM	2751			S 802		28.221						C
ATOM	2752			S 802		29.288				0 26.99 0 29.08		C
MOTA	2753			S 802		28.333						Ŋ
ATOM	2754			S 803		25.978				0 31.09 0 32.53	•	. C
ATOM	2755			S 803		24.853						C
MOTA	2756	6 C	ASN	S 803	•	24.550	24.641	34.497	1.0	0 33.81		C

ATOM	2757	O ASN S 803	23.456	24.143		1.00 34.27
ATOM	2758	CB ASN S 803	23.575	26.659	33.463	1.00 32.29
MOTA	2759	CG ASN S 803	23.640	28.146	33.367	1.00 31.77
MOTA	2760	OD1 ASN S 803	24.688	28.741	33.616	1.00 33.47
	2761	ND2 ASN S 803	22.525	28.772		1.00 29.83
ATOM			25.521	24.015		1.00 35.23
ATOM	2762		25.365	22.689		1.00 36.86
MOTA	2763	CA ALAS 804		-		1.00 37.98
MOTA	2764	C ALAS 804	26.577	22.452		
ATOM	2765	O ALA S 804	27.660	22.949		1.00 37.44
MOTA	2766	CB ALA S 804	25.285	21.610		1.00 36.63
ATOM	2767	N PROS 805	26.394	21.694		1.00 40.20
ATOM	2768	CA PROS 805	27.495	21.381	38.635	1.00 41.46
ATOM	2769	C PROS 805	28.572	20.511	37.983	1.00 42.51
ATOM	2770	O PRO S 805	28.342	19.931.	36.938	1.00 43.07
MOTA	2771	CB PRO S 805	26.799.	20.615	39.774	1.00 41.54
ATOM	2772	CG PRO S 805	25.506	20.116	39.185	1.00 41.29
ATOM	2773	CD PRO S 805	25.117	21.076	38.115	1.00 40.40
ATOM	2774	N ILE S 806	29.728	20.406	38.622	1.00 44.25
MOTA .	2775	CA ILE S 806	30.854	19.627	38.099	1.00 44.96
	2776	C ILE S 806	30.770	18.169	38.532	1.00 45.18
ATOM		O ILE S 806	29.902	17.801	39.323	1.00 45.78
ATOM	. 2777		32.197	20.246	38.569	1.00 45.19
ATOM	2778	CB ILE S 806		20.240	40.070	1.00 46.10
MOTA	2779	CG1 ILE S 806	32.412			1.00 46.10
MOTA	2780	CG2 ILE S 806	32.230	21.743	38.246	
MOTA	2781	CD1 ILE S 806	33.740	20.574	40.597	1.00 46.98
ATOM	2782	N LEU S 812	29.934	8.629	39.561	1.00 43.80
ATOM	2783	CA LEU S 812	29.027	8.736	38.425	1.00 43.90
ATOM	2784	C LEU S 812	29.761	9.243	37.182	1.00 43.45
MOTA	2785	O LEU S 812	30.160	10.410	37.114	1.00 43.36
MOTA	2786	CB LEU S 812	27.862	9.678	38.757	1.00 44.22
ATOM	2787	CG LEU S 812	26.979	9.292	39.951	1.00 45.50
ATOM	2788	CD1 LEU S 812	25.871	10.341	40.144	1.00 46.20
ATOM	2789	CD2 LEU S 812	26.385	7.894	39.793	1.00 45.08
MOTA	2790	N LEUS 813	29.928	8.375	36.190	1.00 42.70
ATOM	2791	CA LEU S 813	30.620	8.776	34.969	1.00 42.21
ATOM	2792	C LEU S 813	29.711	9.604	34.057	1.00 41.46
	27,93		28.492	9.438	34.062	1.00 41.23
ATOM	-		31.167	7.554	34.225	1.00 42.30
ATOM	2794		32.093			1.00 42.35
ATOM	2795		32.494	5.419	34.233	
MOTA	2796			7.398	35.527	1.00 41.80
ATOM	2797		33.322			
MOTA	2798			10.492		
MOTA	2799		29.603	11.385	32.378	1.00 40.26
MOTA	2800		30.475	11.775	31.190	1.00 39.82
MOTA	2801		31.674		31.176	1.00 39.19
MOTA	2802		29.173		33.122	1.00 40.24
ATOM	2803	GG GLN S 814	30.336			1.00 40.51
ATOM	2804		29.879			1.00 41.88
MOTA	2805	OE1 GLN S 814	29.200	14.590	35.419	1.00 41.86
ATOM	2806		30.253	15.919	33.940	1.00 40.63
ATOM	2807		29.864	12.416	30.200	1.00 39.81
MOTA	2808		30.568			1.00 39.53
MOTA	2809		31.402			1.00 39.85
MOTA	2810		30.962			1.00 38.55
ATOM	2811		32.624			1.00 40.44
ATOM	2812		33.553			1.00 41.24
N III OM	2813		33.744			1.00 41.73
. ATOM			33.895			1.00 41.11
MOTA	2814		34.909			1.00 41.24
MOTA	2815		35.752		26.063	
MOTA	2810		37.161		26.019	1.00 43.70
MOTA	281	7 CD GLU S 816	31.101	. 11./90	, 20.019	1.00 40.70

ATOM	2818	OE1	GLU S	816	37.985	11.311	26.814	1.00	45.25		0
MOTA	2819	OE2	GLU S	816	37.447	12.696	25.201	1.00			0
MOTA	2820		GLU S		33.724	10.039	29.479	1.00			N
MOTA	2821		GLU S		33.925	8.877	30.340	1.00			С
MOTA	2822		GLU .		32.744	7.917	30.268	1.00			C
ATOM	2823		GLU S		32.930	6.699	30.252	1.00			0
ATOM	2824		GLU S		34.167	9.308	31.788	1.00			С
ATOM	2825		GLU S		35.463	10.077	31.989	1.00			C
ATOM	2826	CD	GLU S		35.337	11.569	31.688	1.00			0
ATOM	2827		GLU S		34.221 36.362	12.052 12.277	31.394 31.748	1.00	49.02		0
ATOM ATOM	2828 2829	N N		5 817 5 818	31.536	8.470	30.231		44.93		N
ATOM	2830	CA	LEU S		30.335	7.663	30.149		45.78		C
ATOM	2831	C	LEU S		30.359	6.882	28.846		46.89		Ċ
ATOM	2832	Õ	LEU S		30.163	5.663	28.833		46.50		ō
MOTA	2833	СВ	LEU :		29.077	8.537	30.219		45.65		C
ATOM	2834	CG	LEU S		27.741	7.788	30.147		45.58		С
ATOM	2835		LEU :		27.612	6.809	31.318		45.36		С
MOTA	2836	CD2	LEU :		26.551	8.719	30.133	1.00	43.95		С
ATOM	2837	N	LEU :	s 819	30.654	7.588	27.760	1.00	48.01		N
MOTA	2838	CA.		S 819		7.014	26.420		49.24		С
MOTA	2839	C	LEU			5.829	26.247		50.32		С
ATOM	2840	0		S 819		4.777	25.731		50.11		0
MOTA	2841	CB		S 819		8.105	25.380		49.22		C
MOTA	2842	CG		S 819		7.724	23.901		49.32		C
ATOM	2843	CD1				7.178	23.497		48.73		C
MOTA	2844		LEU			8.940	23.058		49.85		C
MOTA	2845	N		S 820		6.005	26.684		51.33 52.53		N C
MOTA	2846	CA	ARG	S 820 S 820		4.966 3.748	26.550 27.414		52.95		c
ATOM .	2847 2848	C O	ARG			2.606	26.942		53.06		Ö
ATOM	2849	СВ	ARG			5.529	26.898		52.91		Č
MOTA	2850	CG		S 820	•	6.583	25.904		54.20		Č
ATOM	2851	CD	ARG			7.046	26.040		55.94		С
ATOM	2852	NE		S 820		8.113	25.081		58.09		N
MOTA	2853	CZ		S 820		8.808	25.022	1.00	59.82		С
MOTA	2854	NH1	ARG	S 820	39.448	8.555	25.867	1.00	60.28		N
MOTA	2855	NH2	ARG	S 820	38.590	9.765	24.108		60.61		N
MOTA	2856	N		S 82		3.994	28.670		53.36		N
MOTA	2857	CA		S 82		2.920	29.561		53.67		С
MOTA	2858	C		S 82			28.892		54.08		C
MOTA	2859	0		S 82		0.862	28.897		54.01		0
ATOM	2860	CB		S 82		3.479	30.883		53.55		C
MOTA	2861	N		S 82			28.308 27.622		54.44 54.93		N C
MOTA	2862	CA C		S 82 S 82			26.398		55.41	•	c
ATOM ATOM	2863 2864	0		S 82			26.143		55.60		o
ATOM	2865	СВ		S 82			27.212		54.90		c
ATOM	2866			S 82			28.361		54.80		Č
MOTA	2867		LEU				27.801		54.39		Ċ
MOTA	2868		LEU				29.335		54.48		C
ATOM	2869			S 82			25.634		55.82		N
ATOM	2870			S 82			24.492		56.04		С
ATOM	2871			S 82			24.901		56.10		С
ATOM	2872			S 82				1.00	56.09		0
MOTA	2873	CB	ASP	S 82	3 31.688		23.320		56.21		С
MOTA	2874	CG		s 82			21.997		56.45		С
MOTA	2875		. ASP				22.028		58.65		0
MOTA	2876		ASP			2.056	20.885	1.00	56.19		0
TER	2877			S 82		07 70-	00.56				E-11
HETAT	м 2878	FE	FE2	A135	0 23.294	27.501	28.594	1.00	20.46		FE

HETATM	2879	C1	OGA	A13	51	22.091	25.173	27.594	1.00	24.79		. C
HETATM	2880	C2	OGA	A13	51	21.066	25.829	28.202	1.00	24.27		С
HETATM	2881	C4	OGA	A13	351	18.756	25.714	29.004	1.00	23.09		C
HETATM		C5	OGA	A13	351	17.415	25.241	28.495	1.00	23.17		С
HETATM		01	OGA			21.909	24.061	27.090		25.24		0
HETATM		02	OGA			23.219	25.658	27.531		24.40		ō
HETATM		02'	OGA.			21.192	26.959	28.711		21.19		ŏ
		03	OGA			16.416	25.662	29.055		23.03		ŏ
HETATM							25.203	28.228		21.70		N
HETATM		N1	OGA			19.886						0
HETATM		04	OGA			17.332	24.475	27.537		23.98		
HETATM		S	SO4			0.316	25.182	43.602		77.77		S
HETATM		01	SO4			1.239	25.980	44.403		77.64		0
HETATM		02	SO4			1.075	24.260	42.760		77.88		0
HETATM	2892	03	SO4			-0.525	24.416	44.514		78.38		0
HETATM	2893	04	SO4	A13	352	-0.507	26.042	42.757		76.90		0
HETATM	2894	S	SO4	A13	353	1.990	28.487	29.834	1.00	69.20		S
HETATM	2895	01	SO4	A1:	353	3.243	29.065	30.309	1.00	68.34		0
HETATM	2896	02	SO4	A1:	353	2.236	27.438	28.847	1.00	67.90		0
HETATM	2897	03	SO4	A1:	353	1.298	27.948	31.009	1.00	70.32		0
HETATM	2898	04	SO4			1.162	29.517	29.203	1.00	69.63	•	0
HETATM		0	нон		1	35.955	31.618	40.285		80.01		0
HETATM		Ö	НОН		2	38.513	33.804	31613		33.04		ō
HETATM		ŏ	НОН		3	36.648	25.786.			76.96		Ö
HETATM		Ö	НОН		4	38.106	25.337	29.179		54.79		ŏ
							30.561	34.967		30.13		Ö
HETATM		0	НОН		5	34.990	•					Ö
HETATM		0	НОН		6	33.934	31.237	38.711		40.66		
HETATM		0	НОН		7	30.766	25.787	37.613		54.75		0
HETATM		0	НОН		8	33.667	28.867	40.196		59.66		0
HETATM		0	нон		9	28.622	27.043	37.556		57.58		0
HETATM	2908	0	НОН		10	19.894	26.655	33.706	1.00	54.88	•	0
HETATM	2909	0	HOH	H	11	30.052	24.213	35.628		41.23		0
HETATM	2910	0	HOH	H	12	28.737	12.960	37.083	1.00	59.80		0
HETATM	2911	0	HOH	H	13	35.568	13.822	23.888	1.00	38.00		0
HETATM	2912	0	HOH	H	14	30.722	-1.323	21.296	1.00	48.92		0
HETATM	2913	0	HOH	Н	15	32.110	2.136	17.673	1.00	69.92		0
HETATM	2914	0	нон	Z	1	9.466	21.720	12.039	1.00	63.79	•	0
HETATM		O	нон		2	1.367	21.270	7.724	1.00	60.01		0
HETATM		Ö	нон		3.	3.426	13.325	8.811		43.04		0
HETATM		ō	НОН		. 4	-0.760	13.029	7.574		47.08	•	0
HETATM		Ö	НОН		5.	2.515	19.304	5.195		46.76		ō
HETATM		ŏ	НОН		6	4.861	33.534	13.331		75.60		Ö
		_			7	1.403	29.250	13.007		46.80		Ö
HETATM		0	НОН				32.100			66.18		o
HETATM			НОН		8	1.614				43.83		0
HETATM		0	HOH		9	12.671	34.540	13.968				
HETATM		0	НОН		10	11.399		. 17.750		68.06		0
HETATM		0	НОН		11	-1.220	30.205	22.820		80.54		0
HETATM		0	НОН		12	6.576	36.529	29.511		43.88		0
HETATM		0	НОН		13	3.525	32.513	31.866		65.87		0
HETATM	2927	0	HOH	Z	14	5.033	37.447	27.566		54.03		0
HETATM	1 2928	0	HOH	Z	15	10.981	35.615			36.24		0
HETATM	1 2929	0	HOH	lZ	16	12.816	42.461	26.787	1.00	37.83		0
HETATM	1 2930	0	HOH	ΙZ	17	13.508	37.138	13.905	1.00	50.79		0
HETATM	1 2931	0	HOH	ΙZ	18	16.409	3.305	16.425	1.00	59.87		0
HETATM			нон		19	14.424				54.39		0
HETATM			НОН		20	11.439				63.10		0
HETATM		ŏ	HOH		21	15.821				43.61		Ō
HETATM			HOH		22	13.496				57.93		ō
HETATM			HOE		23	17.591		•		49.97		ŏ
HETATM			HOE		24	14.617				48.56		Ö
										38.79		0
HETATM			HOH		25	20.840						0
HETATM	2939	Ο.	HOH	1 2	26	27.946	19.151	9.101	Τ.00	3 43.14		O

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F	HETATM	2940	0	нон	Z	27	23.279	21.788	0.672	1.00	62.23			0
	HETATM		0	нон		28	27.443	22.009	43.177	1.00	68.81			0
	ETATM		Ō	НОН		29	27.326	30.900	5.769		84.31			0
	ETATM		Ō	НОН		30	16.938	35.662	41.749		51.88			0
	ETATM		Ö	НОН		31	36.792	29.262	21.033		42.38			ō
	ETATM		0	НОН		32	26.719	37.403	13.167		60.20			ŏ
							29.797	37.403	10.379		60.24			0
	HETATM		0	HOH		33		37.713	15.023		68.08			0
	HETATM		0	НОН		34	28.365							0
	HETATM		0	НОН		35	27.471	34.815	9.298 12.792		63.90			
	HETATM		0	нон		36	.24.262	32.919			45.02		•	0
	HETATM		0	НОН		37	19.704	17.909	13.178		28.78	•		0
	HETATM		0	HOH		38	22.022	12.870	8.792		48.37			0
	HETATM		0	HOH		39	18.151	14.971	12.982		36.76			0
	HETATM		0	нон		40	29.160	5.439	16.977		44.05			0.
	HETATM		0	нон	Z	41	18.863	14.590	16.204		30.84			0
1	HÉTATM	2955	0	НОН		42	12.149	5.293	13.385		72.13			0
1	HETATM	2956	0	HOH	\mathbf{z}	43	15.651	2.782	13.845		41.52			0
1	HETATM	2957	0	HOH	\mathbf{z}	44	14.014	7.467	18.234		52.22			0
1	HETATM	2958	0	HOH	Z	45	5.548	12.548	27.846	1.00	38.03			0
1	HETATM	2959	.0	нон	\mathbf{z}	46	12.742	5.782	36.187	1.00	51.07			0
	HETATM	2960	0	HOH	Z	47	19.063	6.567	36.600	1.00	49.16			0
	HETATM	2961	0	нон	Z	48	19.545	2.633	38.104	1.00	67.28			0
	HETATM			нон		49	7.710	14.276	19.473	1.00	48.41			0
	HETATM			нон		50	15.732	7.234	38.833		54.12	•		0
	HETATM			НОН		51	21.932	13.291	44.351		62.49			Ο.
	HETATM			НОН		52	33.998	44.086	25.334		53.56			0
	HETATM			НОН		53	12.673	21.178	43.612		63.01			0
	HETATM			нон		54	8.172	26.738	44.107		61.46			0
	HETATM			нон		55	9.613	30.854	42.520		54.56			ō
	HETATM			нон		56	13.563	35.806			39.09			ō
•	HETATM			нон		57	15.688	37.473	35.304		47.58			ŏ
	HETATM			нон		58	7.422	43.868	25.982		75.57			ō
	HETATM			НОН		59	7.978	38.223	34.865		59.51			o
						-	16.338	30.836	40.223		38.80			Ö
	HETATM			HOH		60		27.760	38.288		52.22			Ö
	HETATM			HOH		61	17.035				55.16			Ö
	HETATM			НОН		62	22.131		41.390		47.28			0
	HETATM			HOH		63	29.869		39.122					0
	HETATM			HOH		64	28.353		41.766		60.35			Ö
	HETATM	•		НОН		65	31.794		41.962					0
	HETATM			НОН		66	28.058	28.695	48.927		65.95			
	HETATM			HOH		67	24.838	24.783	42.190		52.90			0
	HETATM			HOH		68	11.541		15.082		63.99			0
	HETATM			HOH		69	31.599				44.28			0
	HETATM			HOF		70	24.728				48.25			0
	HETATM			HOH		71	16.271				58.46			0
	HETATM			HOH		72	17.845				57.93			0
	HETATM			HOF		73	16.480				59.15			0
	HETATM			HOH			40.791				58.98			0
	HETATM			HOH	l Z		21.842				67.11			0
	HETATM	1 2989	9 0	HOH			8.791				63.28			0
	HETATM			HOI	ł Z		17.141				52.87			0
	HETATM	1 2991	LO	HOH	H Z	78	21.626	14.804			53.91			0
	HETAT	1 2992	2 0	HO	ı z	79	39.117				57.17			0
	HETATN	1 2993	3 0	HOI	H Z	80	10.617	19.257			69.00			0
	HETATN	1 2994	4 0	HOI	H Z		1.682	24.435	36.842		55.40			0
	HETAT	1 299	5 0	HOI	H Z	82	4.627	30.781	36.487	1.0	53.38			0
	HETATN				H Z		17.463			1.0	38.64			0
	HETATN				ΗZ		18.429				54.65			0
	HETATN				H Z		23.466				0 41.94			0
	HETATI				H Z		26.890				0 49.34			0
	HETATI				H Z		21.694				0 45.95			.0
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HETATM		0	HOH Z	88		9.589	36.847	1.00 5			0
HETATM		0	HOH Z	89	18.447	-1.706	32.981	1.00 6			0
HETATM		0	HOH Z	90	16.300	-0.205	30.017	1.00 5			0
HETATM		0	HOH Z	91	17.950	1.645	20.589	1.00 5			0
HETATM		0	HOH Z	92	26.301	5.439·	16.918	1.00 3			0
HETATM	3006	0	HOH Z.	93	33.944	10.218	13.383	1.00 5		•	0
HETATM	3007	0	HOH Z	94	30.893	16.371	11.174	1.00 4			0
HÉTATM	3008	0	HOH Z	95	32.606	13.689	20.709	1.00 4			0
HETATM	3009	0	HOH Z	96	31.860	10.158		1.00 5	8.55		0
HETATM	3010	0	HOH Z	97	36.957	10.422	7.614	1.00 7		•	0
HETATM	3011	0	HOH Z	98	35.951	16.836	31.735	1.00 5	9.28		0
HETATM	3012	0	HOH Z	99	39.867	18.412	27.150	1.00 5	50.38		0
HETATM	3013	0	HOH Z	100	13.436	20.952	28.355	1.00 2	27.89		0
HETATM	3014	0	HOH Z	101	3.992	21.265	30.540	1.00 4	13.76		0
HETATM	3015	0	HOH Z	102	30.735	37.910	33.103	1.00 3	30.45		0
HETATM	3016	0	HOH Z	103	25.986	26.303	26.047	1.00 2	26.08		0
HETATM	3017.	0	HOH Z	104	36.837	32.025	33.001	1.00 3	37.86		Ο.
HETATM		0	HOH Z		35.845	25.360	27.653	1.00 3	33.53		0
HETATM		0	нон z		31.874	20.474	33.040	1.00 5	55.47		0
HETATM		Ō	HOH Z		36.793	26.619	20.918	1.00	34.57		0
HETATM		0	HOH Z		17.114	16.909					0
HETATM		Ö	HOH Z		9.968	13.510	19.464	-			0
HETATM		ŏ	HOH Z		5.274	16.717	22.023	1.00			0
HETATM		ŏ	HOH Z		7.041	16.862	20.149	1.00			0
HETATM		ŏ	HOH Z		6.517	22.763	22.963	1.00			ō
HETATM		Ö	HOH Z		29.471	38.812	26.249	1.00			ō
HETATM		Ö	HOH Z		32.253	43.121	24.229	1.00			ŏ
HETATM		0	HOH Z		28.797	40.227	16.136	1.00			ŏ
HETATM		Ö	HOH Z		30.645	39.042	18.925	1.00			ŏ
		0			25.466	42.302	17.883	1.00			o
HETATM HETATM		-	HOH Z		27.698	44.486	31.068	1.00			Ö
		0	HOH Z			44.400			38.32		0
HETATM		0	HOH Z		30.274		25.031				0
HETATM		0	HOH Z		27.635	48.525	29.776		35.59		
HETATM		0		121 ·	25.933	50.527	30.463		35.79	•	0
HETATM		0	HOH Z		26.614	31.094	38.158		32.11		0
HETATM		0	HOH Z		29.486	36.934	35.226		27.40	·	.0
HETATM		0	HOH Z		30.510	30.229	36.300		31.99		0
HETATM		0	HOH Z		19.859	31.575	33.786		31.77		0
HETATM		0	HOH Z		18.490	38.301	36.415		43.54		0
HETATM		0	HOH Z		19.538	36.155	33.217		30.91		0
HETATM		0	HOH Z		25.386	44.358	40.124		54.33		0
HETATM		0				42.704			38.88		0
HETATM		0	HOH Z		17.603	37.763	31.961		35.39		0
HETATM		0	HOH Z		9.290	41.007	35.589	•			0
HETATN		Ó	HOH Z		9.348	43.374	27.752		61.17		0
HETATN		0	HOH Z		15.089	37.816	32.481		32.05		0
HETATN	1 3047	0	HOH Z		10.824	48.278	31.295	1.00	52.52		0
HETATI	1 3048	0	HOH Z	135	15.691	44.668	34.824		31.47		0
HETATN	1 3049	0	HOH Z	136	· 15.962	46.870	38.981	1.00	51.42		Ó
HETATI	4 3050	0	HOH Z	137	13.481	51.613	32.894	1.00	45.77		0
HETAT	4 3051	0	HOH Z		14.202	48.658	24.558		43.59		0
HETATI	4 3052	0	HOH Z	139	16.193	44.497	37.574	1.00	58.87		0
HETAT			HOH Z		15.573	46.265	24.419		39.51		0
HETATI			HOH Z		18.684	55.873	28.304		58.28	•	0
HETATI			HOH Z		14.817	55.477	27.388		52.87		0
HETATI			HOH Z		15.284	50.258	22.000		32.96		0
HETATI			HOH Z		23.651	46.151	19.718		33.04		0
HETATI			HOH Z		16.751	46.565	21.800		33.97		0
HETATI			HOH Z		12.595		13.536		39.79		0
HETAT			HOH Z		10.812		14.084		50.88		o
	M .3061		HOH Z		11.495		13.792		44.23		ō
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HOH Z 149 14.521 18.471 12.156 1.00 37.16
HETATM 3062
                  0
                                           33.566 26.082 16.801 1.00 38.34
HETATM 3063
                       HOH Z 150
                                         33.566 26.082 16.601 1.00 36.34

27.798 27.494 24.390 1.00 25.11

30.253 36.176 26.688 1.00 27.79

32.762 34.069 19.065 1.00 47.61

27.363 30.094 25.612 1.00 23.74

16.282 36.168 29.566 1.00 33.13

13.289 26.522 28.472 1.00 47.17
HETATM 3064
                  0
                       HOH Z 151
HETATM 3065
                       HOH Z 152
                  0
HETATM 3066
                       HOH Z 153
                  0
                       HOH Z. 154
HETATM 3067
                  0
HETATM 3068
                  0
                       HOH Z 155
                       HOH Z 156
HETATM 3069
                  0
                                            7.556 30.888
                                                                    24.716 1.00 44.35
                       HOH Z 157
HETATM 3070
                  0
                       HOH Z 158
                                              7.790 30.392
                                                                    27.265 1.00 37.71
HETATM 3071
                  0
                       HOH Z 159
                                             3.910 21.360
                                                                    21.198 1.00 60.23
HETATM 3072
                  0
                                             6.411 23.837
                        HOH Z 160
                                                                    25.422 .1.00 40.51
HETATM 3073
                  0
                                       3.001 17.561 27.759 1.00 55.61 5.352 18.754 24.064 1.00 42.17 40.897 21.985 24.633 1.00 54.83 42.626 37.977 17.732 1.00 71.69 42.463 44.114 19.559 1.00 54.59 33.754 36.855 19.984 1.00 36.17 33.194 39.271 33.406 1.00 28.26 37.482 29.751 37.743 1.00 57.74 38.789 34.566 42.752 1.00 40.46 32.020 40.390 44.008 1.00 38.46 31.865 44.151 45.174 1.00 45.64 41.427 43.475 51.164 1.00 50.64 38.498 47.344 48.085 1.00 60.19 35.239 52.784 45.826 1.00 54.63 32.343 51.933 45.286 1.00 58.03 39.267 57.239 41.745 1.00 26.45 32.755 59.287 44.804 1.00 60.46 46.839 53.182 31.757 1.00 31.38 37.840 55.111 29.241 1.00 44.20
                                              3.001 17.561
                        HOH Z 161
                                                                    27.759
                                                                               1.00 55.61
HETATM 3074
                  0
                        HOH Z 162
HETATM 3075
                  0
                        HOH Z 163
HETATM 3076
                 0
                        HOH Z 164
HETATM 3077
                  0
                  0
                        HOH Z 165
HETATM 3078
                  O HOH Z 166
HETATM 3079
                  O HOH Z 167
HETATM 3080
HETATM 3081
                  O HOH Z 168
                 O HOH Z 169
HETATM 3082
HETATM 3083 O HOH Z 170
HETATM 3084 O HOH Z 171
HETATM 3085 O HOH Z 172
                        HOH Z 173
HETATM 3086 O
                        HOH Z 174
HETATM 3087 O
                        HOH Z 175
HETATM 3088 O
                        HOH · Z 176
 HETATM 3089 O
 HETATM 3090 O HOH Z 177
                        HOH Z 178
 HETATM 3091 O
                         HOH Z 179
 HETATM 3092 O
 CONECT 1478 2878
 CONECT 1498 2878
 CONECT 2167 2878
 CONECT 2878 2885 2884 1478 2167 1498
 CONECT 2879 2880 2883 2884
 CONECT 2880 2879 2885 2887
 CONECT 2881 2882 2887
 CONECT 2882 2881 2886 2888
 CONECT 2883 2879
 CONECT 2884 2879 2878
 CONECT 2885 2880 2878
 CONECT 2886 2882
 CONECT 2887 2880 2881
 CONECT 2888 2882
 CONECT 2889 2890 2891 2892 2893
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  CONECT 2898 2894
                                                                7 6 3090 2
                                                                                            24
                                                 20
                                                         0
                                                                                                   31
  MASTER
                   455
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 END
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Structure 2

Below are the coordinates for structure 2 (the 2.25 Å structure of FIH:Fe(II):20G:CAD):

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12-AUG-02
                                                               1H2L
          TRANSCRIPTION ACTIVATOR/INHIBITOR
HEADER
         FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX WITH HIF-1 ALPHA
TITLE
         2 FRAGMENT PEPTIDE
TITLE
         MOL ID: 1;
COMPND
         2 MOLECULE: FACTOR INHIBITING HIF1;
COMPND
         3 CHAIN: A;
COMPND
         4 ENGINEERED: YES;
COMPND
         5 MOL ID: 2;
COMPND
         6 MOLECULE: HYPOXIA-INDUCIBLE FACTOR 1 ALPHA;
COMPND
         7 SYNONYM: HIF-1 ALPHA, ARNT INTERACTING PROTEIN,
COMPND
        8 MEMBER OF PAS PROTEIN 1;
COMPND
         9 CHAIN: S;
COMPND
COMPND 10 FRAGMENT: C-TERMINAL TRANSACTIVATION DOMAIN FRAGMENT
COMPND 11 RESIDUES 786-826
SOURCE
         MOL_ID: 1;
         2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE
         3 ORGANISM_COMMON: HUMAN;
SOURCE
         4 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE
         5 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE
         6 EXPRESSION SYSTEM PLASMID: PET28A(+);
SOURCE
         7 MOL ID: 2;
SOURCE
         8 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE
        9 ORGANISM_COMMON: HUMAN;
SOURCE
SOURCE 10 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
.SOURCE 11 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
 SOURCE 12 EXPRESSION SYSTEM PLASMID: PGEX-GP-1
           FIH, HIF, DSBH, OXYGENASE, TRANSCRIPTION, HYPOXIA,
 KEYWDS
         2 2-OXOGLUTARATE, ASPARAGINYL HYDROXYLASE, HYDROXYLASE
 KEYWDS
           X-RAY DIFFRACTION
 EXPDTA
           J.M.ELKINS, K.S.HEWITSON, L.A.MCNEILL, I.SCHLEMMINGER,
 AUTHOR
          2 J.F.SEIBEL, C.J.SCHOFIELD
 AUTHOR
              04-SEP-02 1H2L
                                0
 REVDAT
                    J.M.ELKINS, K.S. HEWITSON, L.A. MCNEILL,
 JRNL
             AUTH 2 I.SCHLEMMINGER, J.F. SEIBEL, C.J. SCHOFIELD
 JRNL
                    FIH: HIF-FRAGMENT COMPLEXES
 TRNT
             TTTL
                    TO BE PUBLISHED
 JRNL
             REF
             REFN
 JRNL
 REMARK
          2 RESOLUTION. 2.25 ANGSTROMS.
 REMARK
 REMARK
          3 REFINEMENT.
 REMARK
                           : REFMAC 5.0
              PROGRAM
 REMARK
          3
                           : MURSHUDOV, VAGIN, DODSON
               AUTHORS
 REMARK
           3
 REMARK
           3
                REFINEMENT TARGET : MAXIMUM LIKELIHOOD
 REMARK
           3
  REMARK
           3
              DATA USED IN REFINEMENT.
           3
  REMARK
               RESOLUTION RANGE HIGH (ANGSTROMS) :
                                                      2.25
  REMARK
                                      (ANGSTROMS) :
                                                     38.00
               RESOLUTION RANGE LOW
  REMARK
           3
                                       (SIGMA(F)) : NONE
           3
               DATA CUTOFF
  REMARK
                                              (8):
                                                     99.98
               COMPLETENESS FOR RANGE
  REMARK
                                                      25127
               NUMBER OF REFLECTIONS
  REMARK
  REMARK
           3 FIT TO DATA USED IN REFINEMENT.
  REMARK
                                                 : THROUGHOUT
               CROSS-VALIDATION METHOD
  REMARK
```

```
REMARK
             FREE R VALUE TEST SET SELECTION : RANDOM
         3
         3
             R VALUE (WORKING + TEST SET) : 0.18514
REMARK
                                (WORKING SET) : 0.18253
         3
             R VALUE
REMARK
             FREE R VALUE
         3
                                                 0.21738
REMARK
             FREE R VALUE TEST SET SIZE
REMARK
         3
                                           (왕) : 7.7
                                              : 2104
             FREE R VALUE TEST SET COUNT
REMARK
         3
REMARK
         3
         3
            FIT IN THE HIGHEST RESOLUTION BIN.
REMARK
         3
             TOTAL NUMBER OF BINS USED
                                                         20
REMARK
             BIN RESOLUTION RANGE HIGH
REMARK
REMARK
             BIN RESOLUTION RANGE LOW
REMARK
         3
             REFLECTION IN BIN
                                    (WORKING SET) :
                                                       . 1783
         3
             BIN R VALUE
                                    (WORKING SET) :
REMARK
                                                       0.194
             BIN FREE R VALUE SET COUNT
                                                         170
REMARK
         3
                                                  :
             BİN FREE R VALUE
                                                       0.228
REMARK
         3
         3
REMARK
            NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
         3
REMARK
             PROTEIN ATOMS
                                   : 2863 .
REMARK
         3
                                      : 0
REMARK
         3
             NUCLEIC ACID ATOMS
                                      : 21
REMARK
         3
             HETEROGEN ATOMS
                                    . : 139
REMARK
         3
             SOLVENT ATOMS
REMARK
         3
         3
            B VALUES.
REMARK
                                         (A**2) : NULL
         3
             FROM WILSON PLOT
REMARK
                               (OVERALL, A**2): 27.234
         3
             MEAN B VALUE
REMARK
REMARK
         3
             OVERALL ANISOTROPIC B VALUE.
              B11 (A**2) :
                               -0.40
REMARK
         3
REMARK
         3
              B22 (A**2) :
                               -0.40
REMARK
         3
              B33 (A**2) :
                                0.80
              B12 (A**2) :
REMARK
         3
                               0.00
REMARK
         3
              B13 (A**2) :
                                0.00
              B23 (A**2) :
REMARK
         3
                               0.00
REMARK
         3
         3 ESTIMATED OVERALL COORDINATE ERROR.
REMARK
         3 ESU BASED ON R VALUE
                                                              (A): 0.203
REMARK
                                                              (A): 0.174
REMARK
            ESU BASED ON FREE R VALUE
                                                              (A): 0.165
             ESU BASED ON MAXIMUM LIKELIHOOD
REMARK
            ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2): 6.444
REMARK
 REMARK
 REMARK
          3 CORRELATION COEFFICIENTS.
                                                      0.956
 REMARK
            CORRELATION COEFFICIENT FO-FC
 REMARK
              CORRELATION COEFFICIENT FO-FC FREE:
                                                     0.939
 REMARK
          3 RMS DEVIATIONS FROM IDEAL VALUES
                                               COUNT
                                                          RMS
                                                                 WEIGHT
 REMARK
                                              (A): 2961; 0.013; 0.021
 REMARK
             BOND LENGTHS REFINED
                                              (A): 2961; 0.013; 0.021
 REMARK
              BOND LENGTHS REFINED
                                              (A): 2554; 0.001; 0.020
 REMARK
              BOND LENGTHS OTHERS
                                       (DEGREES): 4026; 1.404; 1.949
              BOND ANGLES REFINED
 REMARK
                                       (DEGREES): 5966; 0.727; 3.000
              BOND ANGLES OTHERS
 REMARK
          3
              TORSION ANGLES, PERIOD 1 (DEGREES):
                                                   350 ; 4.037 ; 3.000
          3
 REMARK
              TORSION ANGLES, PERIOD 3 (DEGREES):
                                                    515 ; 18.189 ; 15.000
          3
 REMARK
              CHIRAL-CENTER RESTRAINTS (A**3):
                                                     413 ; 0.085 ; 0.200
          3
 REMARK
                                                    3315 ; 0.005 ; 0.020
          3
              GENERAL PLANES REFINED
                                              (A):
 REMARK
                                                    602 ; 0.002 ; 0.020
 REMARK
          3
              GENERAL PLANES OTHERS
                                              (A):
              NON-BONDED CONTACTS REFINED (A):
H-BOND (X...Y) REFINED (A):
                                                   693 ; 0.221 ; 0.300
 REMARK
          3
                                                    2483 ; 0.204 ; 0.300
 REMARK
          3
                                                    , 0.156 ; 0.500
16 ; 0.256 ; 0.300
63 ; 0.259
 REMARK
          3
              SYMMETRY VDW REFINED
 REMARK
          3
                                            (A):
              SYMMETRY VDW OTHERS (A):
SYMMETRY H-BOND REFINED (A):
 REMARK
          3
                                                      10 ; 0.200 ; 0.500
 REMARK
          3
 REMARK
```

```
ISOTROPIC THERMAL FACTOR RESTRAINTS. COUNT RMS
REMARK
                                   (A**2): 1767; 0.649; 1.500
           MAIN-CHAIN BOND REFINED
REMARK
           MAIN-CHAIN ANGLE REFINED (A**2): 2847; 1.227; 2.000
REMARK
           SIDE-CHAIN BOND REFINED (A**2): 1194 ; 1.887 ; 3.000
SIDE-CHAIN ANGLE REFINED (A**2): 1179 ; 3.111 ; 4.500
REMARK
REMARK
REMARK
        3
REMARK
        3
          NCS RESTRAINTS STATISTICS
           NUMBER OF NCS GROUPS : NULL
REMARK
        3
REMARK
        3
REMARK
        3 TLS DETAILS
          NUMBER OF TLS GROUPS : 1
REMARK
        3
REMARK
        3
          TLS GROUP: 1
REMARK
        3
          NUMBER OF COMPONENTS GROUP: 2
REMARK
        3
REMARK · 3 COMPONENTS C SSSEQI TO C SSSEQI
                                      A
                            A 15
        3 RESIDUE RANGE :
                                               451
REMARK
        3 RESIDUE RANGE : S
                                 795
                                           S
                                               822
REMARK
        3 ORIGIN FOR THE GROUP (A): 22.2240 27.6230 28.5830
REMARK
REMARK 3 T TENSOR
              T11: 0.1744 T22: 0.0216
REMARK 3
             T33: 0.0949 T12: -0.0059
REMARK 3
              T13: -0.0546 T23: 0.0427
REMARK
        3
        3 L TENSOR
REMARK
            L11: 1.1183 L22: 2.4664
REMARK
REMARK 3 L33:
REMARK 3 L13:
                     1.3415 L12: 0.7934
                    0.5409 L23: 1.2249
REMARK 3 S TENSOR
            S11: 0.0358 S12: -0.1772 S13: -0.0521
REMARK 3
                     0.1763 S22: 0.0025 S23: 0.1089
REMARK 3
               S21:
               S31: 0.2114 S32: -0.0339 S33: -0.0383
REMARK 3
REMARK
        3
REMARK
         3 BULK SOLVENT MODELLING.
REMARK 3 METHOD USED : BABINET MODEL WITH MASK
REMARK 3 PARAMETERS FOR MASK CALCULATION
 REMARK 3 VDW PROBE RADIUS : 1.40
                             : 0.80
 REMARK 3 ION PROBE RADIUS
 REMARK 3 SHRINKAGE RADIUS
                             : 0.80
 REMARK 3
 REMARK .3 OTHER REFINEMENT REMARKS: HYDROGENS HAVE BEEN ADDED IN THE
        3 RIDING POSITIONS
 REMARK
 REMARK
        4 1H2L COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
 REMARK
 REMARK 100
 REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY EBI ON 12-AUG-2002.
 REMARK 100 THE EBI ID CODE IS EBI-11172.
 REMARK 200
 REMARK 200 EXPERIMENTAL DETAILS
                                        : X-RAY DIFFRACTION
 REMARK 200 EXPERIMENT TYPE
                                       : 15-MAY-2002
 REMARK 200
           DATE OF DATA COLLECTION
           TEMPERATURE
                                 (KELVIN) : 100
 REMARK 200
                                     · : 7.5
 REMARK 200 PH
 REMARK 200 NUMBER OF CRYSTALS USED
 REMARK 200
                                    (Y/N) : Y
 REMARK 200 SYNCHROTRON
                                         : SRS BEAMLINE PX14.2
 REMARK 200 RADIATION SOURCE
 REMARK 200 BEAMLINE
                                         : PX14.2
 REMARK 200 X-RAY GENERATOR MODEL
                                        : NULL
 REMARK 200 MONOCHROMATIC OR LAUE
                                 (M/L) : M
 REMARK 200 WAVELENGTH OR RANGE
                                    (A) : 0.983
                                         : NULL
 REMARK 200 MONOCHROMATOR
                                         : NULL
 REMARK 200 OPTICS
```

```
REMARK 200
                                           : CCD
REMARK 200
           DETECTOR TYPE
           DETECTOR MANUFACTURER
                                            : ADSC
REMARK 200
           INTENSITY-INTEGRATION SOFTWARE : MOSFLM
REMARK 200
           DATA SCALING SOFTWARE
                                           : SCALA
REMARK 200
REMARK 200
           NUMBER OF UNIQUE REFLECTIONS
                                           : 27294
REMARK 200
                                       (A) : 2.25
REMARK 200
           RESOLUTION RANGE HIGH
REMARK 200
            RESOLUTION RANGE LOW
                                        (A) : 38.63
REMARK 200
            REJECTION CRITERIA (SIGMA(I)): NONE
REMARK 200
REMARK 200 OVERALL.
                                        (%): 100.0
REMARK 200 COMPLETENESS FOR RANGE
REMARK 200 DATA REDUNDANCY
                                            : 7.0
REMARK 200 R MERGE
                                        (I) : 0.058
REMARK 200 R SYM
                                        (I) : NULL
REMARK 200 <I/SIGMA(I)> FOR THE DATA SET
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.25
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A): 2.37
REMARK 200 COMPLETENESS FOR SHELL (%): 100.0
                                            : 7.2
REMARK 200 DATA REDUNDANCY IN SHELL
                                        (I) : 0.307
REMARK 200 R MERGE FOR SHELL
REMARK 200 R SYM FOR SHELL
                                        (I) : NULL
REMARK 200
            <I/SIGMA(I)> FOR SHELL
                                            : 2.5
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
 REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR REPLACEMENT
 REMARK 200 SOFTWARE USED: NULL
 REMARK 200 STARTING MODEL: NULL
 REMARK 200
REMARK 200 REMARK: NULL
 REMARK 280
 REMARK 280 CRYSTAL
 REMARK 280 SOLVENT CONTENT, VS (%): 63
 REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 3.4
 REMARK 280
 REMARK 280 CRYSTALLIZATION CONDITIONS: 1.2M AMMONIUM SULPHATE, 4% PEG400,
             0.1M HEPES PH7.5, ARGON ATMOSPHERE, 11MG/ML PROTEIN WITH
 REMARK 280
             1MM FE(II), 2.5MM AKG AND 2.5MM PEPTIDE
 REMARK 280
 REMARK 290
 REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
 REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 41 21 2
 REMARK 290
 REMARK 290
                 SYMOP
                         SYMMETRY
 REMARK 290
                MMMMNN
                         OPERATOR
 REMARK 290
                  1555
                         X, Y, Z
                  2555
                         -X, -Y, 1/2+Z
 REMARK 290
 REMARK 290
                  3555
                         1/2-Y, 1/2+X, 1/4+Z
 REMARK 290
                  4555
                         1/2+Y, 1/2-X, 3/4+Z
                  5555
                         1/2-X, 1/2+Y, 1/4-Z
 REMARK 290
                         1/2+X, 1/2-Y, 3/4-Z
 REMARK 290
                   6555
                  7555
 REMARK 290
                         Y, X, -Z
                  8555
 REMARK 290
                         -Y, -X, 1/2-Z
 REMARK 290
                WHERE NNN -> OPERATOR NUMBER
 REMARK 290
                      MMM -> TRANSLATION VECTOR
 REMARK 290
 REMARK 290
 REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
 REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
```

```
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
                                                                                                                     0.00000
                        SMTRY1
                                          1 1.000000 0.000000 0.000000
REMARK 290
                                          1 0.000000 1.000000 0.000000
                                                                                                                    0.00000
                        SMTRY2
REMARK 290
                      SMTRY3 1 0.000000 0.000000 1.000000
                                                                                                                    0.00000
REMARK 290 SMTRY1 2 -1.000000 0.000000 0.000000 REMARK 290 SMTRY1 2 -1.000000 0.000000 0.000000 0.000000 REMARK 290 SMTRY2 2 0.000000 -1.000000 0.000000 REMARK 290 SMTRY3 2 0.000000 -1.000000 0.000000 REMARK 290 SMTRY1 3 0.000000 -1.000000 0.000000 REMARK 290 SMTRY2 3 1.000000 0.000000 0.000000 REMARK 290 SMTRY3 3 0.000000 0.000000 0.000000 REMARK 290 SMTRY1 4 0.000000 0.000000 0.000000 REMARK 290 SMTRY1 4 0.000000 0.000000 0.000000 REMARK 290 SMTRY2 4 -1.000000 0.000000 0.000000 REMARK 290 SMTRY2 5 -1.000000 0.000000 0.000000 REMARK 290 SMTRY3 5 0.000000 0.000000 0.000000 REMARK 290 SMTRY3 5 0.000000 0.000000 0.000000 REMARK 290 SMTRY3 5 0.000000 0.000000 0.000000 REMARK 290 SMTRY3 6 0.000000 0.000000 0.000000 REMARK 290 SMTRY3 6 0.000000 0.000000 0.000000 REMARK 290 SMTRY3 6 0.000000 0.000000 0.000000 REMARK 290 SMTRY3 6 0.000000 0.000000 0.000000 REMARK 290 SMTRY3 6 0.000000 0.000000 0.000000 REMARK 290 SMTRY3 6 0.000000 0.000000 0.000000 REMARK 290 SMTRY3 7 0.000000 0.000000 0.000000 REMARK 290 SMTRY3 7 0.000000 0.000000 -1.000000 REMARK 290 SMTRY3 7 0.000000 0.000000 -1.000000 REMARK 290 SMTRY3 8 0.000000 -1.000000 0.000000 REMARK 290 SMTRY3 8 0.000000 -1.000000 0.000000 REMARK 290 SMTRY3 8 0.000000 0.000000 -1.000000 REMARK 290 SMTRY3 8 0.000000 0.000000 -1.000000 REMARK 290 SMTRY3 8 0.000000 0.000000 -1.000000  -1.000000 -1.000000 REMARK 290 SMTRY3 8 0.0000000 0.000000 -1.000000
REMARK 290
                       SMTRY1 2 -1.000000 0.000000 0.000000
                                                                                                                    0.00000
                                                                                                                   73.95700
                                                                                                                   43.13200
                                                                                                                    43.13200
                                                                                                                    36.97850
                                                                                                                   43.13200
                                                                                                                    43.13200
                                                                                                                 110.93550
                                                                                                                   43.13200
                                                                                                                    43.13200
                                                                                                                    36.97850
                                                                                                                    43.13200
                                                                                                                     43.13200
                                                                                                                  110.93550
                                                                                                                     0.00000
                                                                                                                       0.00000
                                                                                                                       0.00000
                                                                                                                      0.00000
                                                                                                           0.00000
73.95700
 REMARK 290
 REMARK 290 REMARK: NULL
 REMARK 300
 REMARK 300 BIOMOLECULE: 1
 REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
 REMARK 300 WHICH CONSISTS OF 2 CHAIN(S). SEE REMARK 350 FOR
  REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
  REMARK 300
  REMARK 300 QUATERNARY STRUCTURE FOR THIS ENTRY: TETRAMERIC
  REMARK 300
  REMARK 300 THE PROTEIN IS A HOMODIMER FORMED BY CHAIN A.
  REMARK 300 A HETERODIMERIC ASSOCIATION OF CHAIN A WITH CHAIN S
  REMARK 300 PRODUCES A TETRAMER.
  REMARK 300
  REMARK 300 THE BURIED SURFACE AREA SHOWN BELOW IS AN AVERAGE
  REMARK 300 CALCULATED FOR THE HETEROTETRAMER AND DOES NOT
  REMARK 300 CORRESPOND TO THE BURIED SURFACE AREA FOR THE
  REMARK 300 HOMODIMER OF CHAIN A
  REMARK 300
  REMARK 300 THE HETERO-ASSEMBLY DESCRIBED BY REMARK 350 APPEARS
   REMARK 300 TO BE A CASE OF STRONG CRYSTAL PACKING WITH
   REMARK 300 THE MEAN DIFFERENCE IN ACCESSIBLE SURFACE AREA PER
   REMARK 300 CHAIN BETWEEN THE ISOLATED CHAIN AND THAT FOR
   REMARK 300 THE CHAIN IN THE COMPLEX IS 2141.3 ANGSTROM**2
   REMARK 350
   REMARK 350 GENERATING THE BIOMOLECULE
   REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
   REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
   REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
   REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND
   REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
   REMARK 350
   REMARK 350 BIOMOLECULE: 1
    REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, S
    REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000
```

```
REMARK 350
             BIOMT2
                          0.000000
                                     1.000000
                                                0.000000
                                                                  0.00000
REMARK 350
             BIOMT3
                       1
                          0.000000
                                     0.000000
                                                1.000000
                                                                  0.00000
                       2
REMARK 350
             BIOMT1
                          0.000000 -1.000000
                                                0.000000
                                                                 86.26400
REMARK 350
             BIOMT2
                       2 -1.000000
                                     0.000000
                                                0.000000
                                                                 86.26400
REMARK 350
             BIOMT3
                       2
                          0.000000
                                     0.000000 -1.000000
                                                                 73.95700
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
REMARK 465
              M RES C SSSEQI
REMARK 465
               MET A
                           1
REMARK 465
                ALA A
                           2
REMARK 465
                ALA A
                           3
REMARK 465
                THR A
                           4
REMARK 465
                ALA A
                           5
REMARK 465
                ALA A
                           6
                           7
REMARK 465
                GLU A .
REMARK 465
                ALA A
                           8
REMARK 465
                VAL A
                           9
REMARK 465
                ALA A
                          10
REMARK 465
                SER A
                         11
REMARK 465
                GLY A
                          12
REMARK 465
                SER A
                          13
REMARK 465
                GLY A
                         14
REMARK 465
                LYS A
                         304
REMARK 465
                ARG A
                         305
REMARK 465
                ILE A
                         306
REMARK 465
                SER S
                         786
REMARK 465
                MET S
                         787
REMARK 465
                ASP S
                         788
REMARK 465
                GLU S
                         789
REMARK 465
                SER S
                         790
REMARK 465
                GLY S
                         791
REMARK 465
                LEU S
                         792
REMARK 465
                PRO S
                         793
REMARK 465
                GLN S
                         794
REMARK 465
                GLN S
                         807
REMARK 465
                GLY S
                         808
REMARK 465
                SER S
                         809
REMARK 465
                ARG S
                         810
REMARK 465
                ASN S
                         811
REMARK 465
                LEU S
                         812
REMARK 465
                ASP S
                         823
REMARK 465
                GLN S
                         824
REMARK 465
                VAL S
                         825
REMARK 465
                ASN S
                         826
REMARK 470
REMARK 470 MISSING ATOM
REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;
REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;
REMARK 470 I=INSERTION CODE):
REMARK 470
              M RES CSSEQI
                             ATOMS
REMARK 470
                GLU A
                       15
                              CG
                                    CD
                                         OE1
                                               OE2
REMARK 470
                GLU A
                        29
                              CG
                                    CD
                                         OE1
                                               OE<sub>2</sub>
REMARK 470
                ASN A 87
                              CG
                                    OD1
                                         ND2
                LYS A 106
REMARK 470
                              CD
                                    CE
                                         NZ
                                               CZ
REMARK 470
                ARG A 117
                              CG
                                    CD
                                         NE
                                                    NH1
                                                          NH2
REMARK 470
                GLN A 133
                              CG
                                    CD
                                               NE2
                                         OE1
REMARK 470
                GLN A 136
                              CG
                                    CD
                                         OE1
                                               NE2
```

```
GLN A 137 CG CD
                                     OE1 NE2
 REMARK 470
                                               NH1 NH2
              ARG A 156
                            CG CD
                                     NE
 REMARK 470
                                     NZ
                                CE
 REMARK 470
               LYS A 157
                            CD
                                      CE
                                          NZ
 REMARK 470
              LYS A 311
 REMARK 500
 REMARK 500 GEOMETRY AND STEREOCHEMISTRY
 REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
 REMARK 500
 REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
 REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
 REMARK 500 THAN 6*RMSD AND BY MORE THAN 0.150 ANGSTROMS (M=MODEL
 REMARK 500 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
 REMARK 500 NUMBER; I=INSERTION CODE).
. REMARK 500
 REMARK 500 STANDARD TABLE:
 REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 1X, 2(A4, A1, 3X), 12X, F5.3)
 REMARK 500
 REMARK 500 EXPECTED VALUESS: ENGH AND HUBER, 1991
 REMARK 500
 REMARK 500 M RES CSSEQI ATM1 RES CSSEQI ATM2 DEVIATION
                                MET A 343 ČE
                                                 -0.243
             MET A 343 SD
  REMARK 500
  REMARK 500
  REMARK 500 REMARK: NULL
  REMARK 500
  REMARK 500 GEOMETRY AND STEREOCHEMISTRY
  REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
  REMARK 500
  REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
  REMARK 500
                                                             DISTANCE
  REMARK 500 ATM1 RES C SSEQI ATM2 RES C SSEQI
  REMARK 500
              O ALA A 300 OH TYR S 798
                                                                 2.18
  REMARK 500
  REMARK 525
  REMARK 525 SOLVENT
  REMARK 525
  REMARK 525 THE SOLVENT MOLECULES ARE GIVEN CHAIN IDENTIFIERS TO
  REMARK 525 INDICATE THE PROTEIN CHAIN TO WHICH THEY ARE MOST CLOSELY
  REMARK 525 ASSOCIATED WITH:
  REMARK 525 PROTEIN CHAIN SOLVENT CHAIN
  REMARK 525 A
                              Z
  REMARK 525
                               Н
  REMARK 600
  REMARK 600 HETEROGEN
  REMARK 600
  REMARK 600 FOR METAL ATOM FE FE2 A1350 THE COORDINATION ANGLES ARE:
  REMARK 600 1 HIS 199A NE2
                                    103.4
  REMARK 600 2 ASP
                    201A OD2
                    279A NE2
                                     83.1 86.0
  REMARK 600 3 HIS
                                     168.9 87.6 98.2
  REMARK 600 4 AKG 1351A 01
                                    87.0 169.4 97.2 81.9
   REMARK 600 5 AKG 1351A 05
                                        1
                                                  3
   REMARK 600
   REMARK 700
   REMARK 700 SHEET
   REMARK 700 THE SHEET STRUCTURE OF THIS MOLECULE IS BIFURCATED. IN
   REMARK 700 ORDER TO REPRESENT THIS FEATURE IN THE SHEET RECORDS BELOW,
   REMARK 700 TWO SHEETS ARE DEFINED.
   REMARK 800
   REMARK 800 SITE
   REMARK 800 SITE IDENTIFIER: FE1
   REMARK 800 SITE DESCRIPTION: FE BINDING SITE FOR CHAIN A
   REMARK 800
```

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REMARK 800 SITE_IDENTIFIER: AKG
REMARK 800 SITE DESCRIPTION: AKG BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE IDENTIFIER: SO1
REMARK 800 SITE DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE IDENTIFIER: SO2
REMARK 800 SITE DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 1D7G
                            RELATED DB: PDB
REMARK 900 A MODEL FOR THE COMPLEX BETWEEN THE
REMARK 900
           HYPOXIA-INDUCIBLE FACTOR-1 (HIF-1) AND ITS
REMARK 900
            CONSENSUS DEOXYRIBONUCLEIC ACID SEQUENCE
REMARK 900 RELATED ID: 1H2K
                            RELATED DB: PDB
REMARK 900
           FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900
           WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1H2M
                             RELATED DB: PDB
           FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900
REMARK 900
           WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1H2N
                            RELATED DB: PDB
REMARK 900
           FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900
           WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1L8C RELATED DB: PDB
REMARK 900
           STRUCTURAL BASIS FOR HIF-1ALPHA/CBP
           RECOGNITION IN THECELLULAR HYPOXIC RESPONSE
REMARK 900
REMARK 900 RELATED ID: 1LM8 RELATED DB: PDB
REMARK 900
           STRUCTURE OF A HIF-1A-PVHL-ELONGINB-
REMARK 900
           ELONGINC COMPLEX
REMARK 900 RELATED ID: 1LQB
                              RELATED DB: PDB
REMARK 900
           CRYSTAL STRUCTURE OF A HYDROXYLATED HIF-1
REMARK 900
            ALPHA PEPTIDEBOUND TO THE PVHL/ELONGIN-C/
REMARK 900
           ELONGIN-B COMPLEX
                                          096907
DBREF
       1H2L A
                1 349 SWS
                                 Q969Q7
                     826 SWS
               786
DBREF
       1H2L S
                               . Q16665
                                          HIFA HUMAN
                                                         786
                                                                 826
SEORES
         1 A
              349
                  MET ALA ALA THR ALA ALA GLU ALA VAL ALA SER GLY SER
SEQRES
         2 A
              349
                   GLY GLU PRO ARG GLU GLU ALA GLY ALA LEU GLY PRO ALA
SEQRES
         3 A
                   TRP ASP GLU SER GLN LEU ARG SER TYR SER PHE PRO THR
              349
SEQRES
         4 A
              349
                   ARG PRO ILE PRO ARG LEU SER GLN SER ASP PRO ARG ALA
                   GLU GLU LEU ILE GLU ASN GLU GLU PRO VAL VAL LEU THR
SEQRES
         5 A
              349
SEQRES
         6 A
              349
                   ASP THR ASN LEU VAL TYR PRO ALA LEU LYS TRP ASP LEU
SEQRES .
         7 A
              349
                   GLU TYR LEU GLN GLU ASN ILE GLY ASN GLY ASP PHE SER
         8 A.
SEQRES
              349
                   VAL TYR SER ALA SER THR HIS LYS PHE LEU TYR TYR ASP
SEORES
         9 A
              349
                   GLU LYS LYS MET ALA ASN PHE GLN ASN PHE LYS PRO ARG
SEORES
        10 A
              349
                   SER ASN ARG GLU GLU MET LYS PHE HIS GLU PHE VAL GLU
SEQRES
        11 A
              349
                   LYS LEU GLN ASP ILE GLN GLN ARG GLY GLY GLU GLU ARG
SEORES
        12 A
              349
                   LEU TYR LEU GLN GLN THR LEU ASN ASP THR VAL GLY ARG
SEORES
        13 A
              349
                   LYS ILE VAL MET ASP PHE LEU GLY PHE ASN TRP ASN TRP
SEQRES
        14 A
              349
                   ILE ASN LYS GLN GLN GLY LYS ARG GLY TRP GLY GLN LEU
SEQRES
        15 A
              349
                   THR SER ASN LEU LEU LEU ILE GLY MET GLU GLY ASN VAL
SEORES
        16 A
              349 THR PRO ALA HIS TYR ASP GLU GLN GLN ASN PHE PHE ALA
SEQRES
        17 A
              349
                   GLN ILE LYS GLY TYR LYS ARG CYS ILE LEU PHE PRO PRO
SEQRES
        18 A
              349
                   ASP GLN PHE GLU CYS LEU TYR PRO TYR PRO VAL HIS HIS
SEORES
        19 A
              349
                   PRO CYS ASP ARG GLN SER GLN VAL ASP PHE ASP ASN PRO
SEORES
        20 A
              349
                   ASP TYR GLU ARG PHE PRO ASN PHE GLN ASN VAL VAL GLY
SEQRES
        21 A
              349
                   TYR GLU THR VAL VAL GLY PRO GLY ASP VAL LEU TYR ILE
SEORES
        22 A
              349
                   PRO MET TYR TRP TRP HIS HIS ILE GLU SER LEU LEU ASN
SEQRES
        23 A
              349
                   GLY GLY ILE THR ILE THR VAL ASN PHE TRP TYR LYS GLY
SEQRES
        24 A
                   ALA PRO THR PRO LYS ARG ILE GLU TYR PRO LEU LYS ALA
              349
SEORES
       25 A 349
                   HIS GLN LYS VAL ALA ILE MET ARG ASN ILE GLU LYS MET
SEQRES 26 A 349 LEU GLY GLU ALA LEU GLY ASN PRO GLN GLU VAL GLY PRO
```

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27 A 349 LEU LEU ASN THR MET ILE LYS GLY ARG TYR ASN
SEORES
                  SER MET ASP GLU SER GLY LEU PRO GLN LEU THR SER TYR
        1 S
               41
SEQRES
                   ASP CYS GLU VAL ASN ALA PRO ILE GLN GLY SER ARG ASN
               41
SEQRES
         2 S
                   LEU LEU GLN GLY GLU GLU LEU LEU ARG ALA LEU ASP GLN
         3 S
               41
SEORES
                   VAL ASN
SEQRES
         4 S
               41
                    · 1
           A1350
       FE2
                       10
       AKG
           A1351
HET
                        5
       SO4
           A1352
HET
       SO4 A1353
                        5
HET
           FE2 FE (II) ION
HETNAM
HETNAM
           AKG 2-OXYGLUTARIC ACID
HETNAM
           SO4 SULFATE ION
            FE2
                   FE1 2+
FORMUL
         3
                   C5 H6 O5
            AKG
FORMUL
         4
            SO4
                   2(O4 S1 2-)
         5
FORMUL
            HOH
                  *139(H2 O1)
         6
FORMUL
                                                                              5
             1 ASP A
                       28
                           LEU A
                                    32
                                        5
HELIX
         1
                                                                             10
         2
             2 ASP A
                        49
                            ASN A
                                    58
                                        1
HELIX
                                                                              7
                        70
                                    76
                                        5
HELIX
         3
             3 VAL A
                            TRP A
                        77
                            ILE A
                                    85
                                        1
HELIX
         4
             4 ASP A
                                         5
                       104
                            PHE A
                                   111
             5 ASP A
HELIX
         5
                                                                             15
                                   138
             6 LYS A
                       124
                            ARG A
                                        1
HELIX
         6
                                                                             10
                                   164
             7 GLY A
                       155
                            GLY A
                                         1
HELIX
         7
                                                                             13
                            GLY A
                                   178
                                         1
HELIX
         8
             8 ASN A
                       166
HELIX
         9
             9 PRO A
                       220
                            ASP A
                                   222
                                         5
                                   228
HELIX
        10
            10 GLN A
                       223
                            TYR A
                                         1
                                   258
             11 PHE A
                       252
                            VAL A
                                         5
HELIX
        11
                                                                              21
             12 LYS A
                       311
                            GLY A
                                   331
                                         1
HELIX
        12
             13 ASN A
                       332
                            GLN A
                                   334
                                         5
HELIX
        13
                                                                              11
             14 GLU A
                       335
                            LYS A
                                   345
                                         1
HELIX
         14
HELIX
         15
             15 GLN S
                       814
                            LEU S 822
                                         1
        . 1
             AA 5 THR A 39
                             PRO A 41
                                         0
SHEET
                                                               ARG A 40
             AA 5 GLY A 260
                                               GLY A 260
                                                           N
 SHEET
          2
                             VAL A 265
                                        1
                                            0
                                                               VAL A 265
            AA 5 LYS A 214
                             PHE A 219 -1
                                            O.
                                               LYS A 214
                                                            N
 SHEET
          3
                                                               PHE A 219
                             SER A 283 -1
                                               TRP A 278
                                                            Ν
 SHEET
          4
            AA 5 TRP A 278
                                            Ω
                                               THR A 196
                                                            Ν
                                                               ILE A 281
          5
            AA 5 VAL A 195
                             HIS A 199 -1
 SHEET
            AB 6 ARG A 44
                             LEU A 45
                                        0
 SHEET
          1
                                                                      45
                                               VAL A 63
                                                            N
                                                               LEU A
 SHEET
          2
            AB 6 VAL A 62
                             LEU A 64 1
                                            0
                                                               LEU A 64
                                               VAL A 270
                                                            N
             AB 6 VAL A 270
                             ILE A 273 -1
                                            0
 SHEET
          3
                                                               ILE A 273
                                               ASN A 205
                                                            N
             AB 6 GLN A 204 LYS A 211 -1
                                            0
 SHEET
          4
                                               ILE A 291
                                                               ILE A 210
          5 AB 6 THR A 290 TYR A 297 -1
                                            0
                                                            N
 SHEET
                             SER A 184 -1
                                            N
                                               THR A 183
                                                               TRP A 296
          6 AB 6 LEU A 182
 SHEET
                             LEU A 45 0
          1 AC 9 ARG A 44
 SHEET
                                                               LEU A 45
          2 AC 9 VAL A 62
                              LEU A 64 1
                                            0
                                               VAL A 63
                                                            N
 SHEET
                                                            N
                                                               LEU A 64
                              ILE A 273 -1
                                            0
                                               VAL A 270
          3 AC 9 VAL A 270
 SHEET
                                               ASN A 205
                                                               ILE A 273
                                            0
                                                            N
          4 AC 9 GLN A 204
                              LYS A 211 -1
 SHEET
                                               ILE A 291
                                                               ILE A.210
                              TYR A 297 -1
                                            0
                                                            N
          5 AC 9 THR A 290
 SHEET
                                                               ASN A 294
          6 AC 9 LEU A 186 GLY A 190 -1
                                            0
                                               LEU A 186.
                                                            N
 SHEET
                              THR A 149 -1
                                               LEU A 146
                                                            N
                                                               ILE A 189
          7 AC 9 ARG A 143
                                            0
 SHEET
                                                               GLN A 147
                                             O . SER A 91
            AC 9 PHE A 90
                              ALA A 95 -1
                                                            N
          8
 SHEET
                                                               SER A
            AC 9 SER A 118
                              MET A 123 -1
                                             O ASN A 119
                                                            N
 SHEET
                                                                1555
                                                                        1555
 LINK
             FE
                   FE2 A1350
                                             NE2 HIS A 199
                                                                1555
                                                                        1555
                                              OD2 ASP A 201
 LINK
             FE
                   FE2 A1350
                                                                1555
                                                                        1555
                                              NE2 HIS A 279
             FE
                   FE2 A1350
 LINK
                                                                        1555
                                              01 AKG A1351
                                                                1555
                   FE2 A1350
             FE
 LINK
                                              05 AKG A1351
                                                                1555
                                                                        1555
                   FE2 A1350
 LINK
             FE
          1 TYR A 308
                          PRO A 309
                                                0
                                                          1.27
 CISPEP
          1 FE1 3 HIS A 199
                              ASP A 201
                                          HIS A 279
 SITE .
                               THR A 196
                                           HIS A 199
                                                      ASP A 201
          1 AKG 12 TYR A 145
 SITE
          2 AKG 12 ASN A 205 PHE A 207
                                           LYS A 214
                                                      HIS A 279
 SITE
          3 AKG 12 ILE A 281 ASN A 294
                                           TRP A 296
                                                     HOH Z 65
 SITE
```

8

3

6

7

3

SITE	1 SC	1 4	ARG	Α	138 GT	LY A 140	GLU A 14	11 GLU <i>I</i>	142			
SITE	1 SC		ARG			LU A 192	GLY A 19					
SITE	2 SC		ASN									
CRYST1	86.2	64	86.			914 90.00	90.00	90.00	P 41 2	1 2	8	
ORIGX1		000			000000	0.00000		0.00000				•
ORIGX2		0.000			000000	0.00000		0.00000				
ORIGX3		0.000			000000	1.00000		0.00000				
SCALE1		0.011			000000	0.00000		0.00000				
SCALE2		0.000			011592	0.00000		0.00000				
SCALE3		0.000			.000000	0.00676		0.00000	1 00	61 70		
ATOM	. 1		GLU		15 15	8.505	32.866 32.223	9.893		61.72		N
ATOM ATOM	2 3		GLU GLU		15 15	7.173 7.251	32.223	9.682 10.070		61.95 61.54		. c
ATOM	4		GLU		15	8.109	30.749	9.581		61.66		0
ATOM	5		GLU		15	6.724	32.375	8.234		62.08		C
ATOM	6		PRO		16	6.353	30.305	10.941		61.24		N
ATOM	7		PRO		16	6.386	28.928	11.455	1.00	60.97		C
ATOM	8		PRO		16	6.342	27.853	10.368		60.27		C
ATOM	9	0	PRO	Α	16	5.494	27.879	9.479		60.01		0
ATOM	10	СВ	PRO	A	16	5.134	28.849	12.333	1.00	61.10		С
MOTA	11	CG	PRO	Α	16	4.790	30.262	12.653		61.53	•	С
ATOM	12	CD	PRO		16	5.228	31.079	11.488	1.00			С
MOTA	13	N	ARG		17	7.256	26.900	10.464		59.45		N
ATOM	14	CA	ARG		17	7.348	25.820	9.494		59.05		C
ATOM	15	C	ARG		17	6.083	24.971	9.478		57.86		C
MOTA	16	0	ARG		17	5.312	24.963	10.437		57.86		0
ATOM	17 18	CB	ARG		17 17	8.541	24.913	9.827 9.859		59.53		C
MOTA MOTA	19	CG CD	ARG ARG		17	9.906 11.080	25.621 24.696	10.194	1.00	60.69 62.32		C
ATOM	20	NE	ARG		17	11.040	24.185	11.567		63.73		N
ATOM	21	CZ	ARG		17	11.464	24.852	12.649		65.28		C
ATOM	22		ARG		17	11.962	26.085	12.544		65.01		N
ATOM	23		ARG		17	11.385	24.282	13.848		65.09		N
ATOM	24	N	GLU		18	5.878	24.254	8.382		56.26		N
ATOM	25	CA	GLU	A	18	4.749	23.351	8.273	1.00	55.12		C
ATOM	26	С	GLU	A	18	5.222	21.931	8.587	1.00	53.54		С
MOTA	27	0	GLU		18	6.214	21.468	8.031		52.86		0
ATOM	28	CB	GLU		18	4.150	23.406	6.867		55.33		C
MOTA	29	CG	GLU		18	3.482	24.731	6.519		56.39		С
ATOM	30	CD	GLU		18	2.100	24.904	7.137		57.19		C
ATOM	31		GLU		18	1.559	23.935	7.718		56.35	-	0
ATOM ATOM	32 33	N N	GLU GLU		18 19	1.548 4.526	26.023 21.260	7.028 9.501		58.12 51.73		N N
MOTA	34	CA	GLU		19	4.823	19.867	9.816		50.56		C
ATOM	35	C	GLU		19	4.409	18.944	8.663		48.36		Ċ
ATOM	36	ō	GLU		19	3.312	19.066	8.102		47.54		Ö
ATOM	37	СВ	GLU		19	4.115	19.422	11.100		51.05		C
ATOM	38	CG	GLU		19	4.577	20.139	12.360		53.53		С
MOTA	39	CD	GLU	A	19	4.363	19.323	13.638	1.00	57.67		С
ATOM	40		GLU		19	3.906	18.146	13.561		59.24		0
ATOM	41		GLU		19	4.663	19.864	14.735		59.50		0
ATOM	42	N	ALA		20	. 5.314	18.035	8.320		46.04		N
ATOM	43	CA	ALA		20	5.100	17.030	7.283		44.66		C
MOTA	44	С	ALA		20	3.741	16.365	7.394		42.92		C
ATOM	45 46	O	ALA		20	3.230	16.154	8.491		42.14		0
ATOM ATOM	46 47	CB N	ALA GLY		20 21	6.182 3.173	15.965 16.025	7.360 6.247		44.46 41.16		C N
ATOM	48	CA	GLY		21	1.897	15.341	6.247		40.22		C
ATOM	49	C	GLY		21	0.757	16.300	6.480		39.27		, C
ATOM	50	Õ	GLY		21	-0.309	15.895	6.908		38.03		. 0
MOTA	51	N	ALA		22	1.005	17.584	6.240		38.86		N

ATOM	52 C	ALA A	Α	22			18.611	6.371	1.00 38	3.79		С
ATOM	53 C	ALA	A	22			18.613	7.758	1.00 38	3.64	•	С
ATOM	54 O	ALA		22			18.759	7.924	1.00 38		•	0
ATOM	55 CI			22		-1.102	18.409	5.324	1.00 38			C
ATOM	56 N	LEU		23		0.231	18.451	8.760	1.00 39			N
ATOM	57 C			23		-0.233	18.473		1.00 39		•	C
MOTA	58 C	LEU		23		-0.290	19.886	10.692	1.00 3			C
MOTA	59 O			23		-0.464	20.075	11.880	1.00 3			0
ATOM	60 C			23		0.642	17.574	11.003	1.00 40			C
ATOM	61 C			23		0.528	16.118	10.558	1.00 4			C C
MOTA		D1 LEU		23		1.414	15.185	11.384	1.00 4			C
ATOM		D2 LEU		23		-0.916	15.673	10.633	1.00 4			N
ATOM .	64 N			24		-0.156	20.879 22.258	9.823 10.237	1.00 3			C
MOTA	65 C			24		-0.290 0.964	22.236	10.237	1.00 3			Č
ATOM	66 C 67 O			24 24		2.011	22.219	10.820	1.00 3			ŏ
ATOM	67 O 68 N			·25		0.854	24.118	11.223	1.00 3			N
ATOM		A PRO		25		1.997	24.830	11.775	1.00 3			Ċ
ATOM ATOM	70 C			25		2.410	24.197	13.086		8.68		C
ATOM	71 0			25		1.572	23.842	13.914	1.00 3			0
. ATOM		B PRO		25		1.477	26.259	12.001	1.00 3			С
ATOM		G PRO		25		-0.004	26.197	11.895	1.00 3		•	С
ATOM		D PRO		25		-0.375	24.930	11.210	1.00 3	9.17		C ·
ATOM	75 N			26		3.713	24.037	13.246	1.00 3	8.92		N
ATOM		A ALA		26		4.269	23.489	14.467	1.00 3	39.38		С
ATOM	77 (26		3.924	24.381	15.676	1.00 3			C
MOTA	. 78 C) ALA	A	26		3.677	23.882	16.772	1.00 3			0
MOTA	79 (CB ALA	A	26		5.762	23.347	14.319	1.00 3			C,
MOTA	80 1	I TRE	A	27		3.871	25.687	15.468	1.00 3	•		N
MOTA	81 (CA TRE		27		3.516	26.602	16.543	1.00 3			C
MOTA	82 (TRE		27		3.034	27.919	15.941	1.00 3			C
MOTA			? A	27		3.013	28.074	14.731	1.00			0
MOTA			? A	27	•	4.746	26.835	17.424	1.00			C C
MOTA			P A	27		5.949	27.019	16.596	1.00			C.
ATOM			? A	27		6.770	26.041	16.089	1.00			C
MOTA			PA	27		6.450	28.249	16.107 15.324	1.00			N
ATOM			PA	27 27		.7.761 7.592	26.610 27.966	15.324	1.00			C
ATOM			PA	27		6.066	29.568	16.263	1.00			Č
MOTA			PA PA	27		8.332	28.947	14.720	1.00			Č
MOTA			PA	27		6.808	30.539	15.664	1.00			Ċ
ATOM ATOM		CH2 TR		27		7.927	30.225	14.890	1.00			С
ATOM			P A	28		2.620	28.860	16.775	1.00			N
ATOM			PA	28		2.253	30.168	16.267	1.00			С
ATOM			P A	28		2.816	31.224	17.160	1.00			С
ATOM			P A	28		3.311	30.948	18.250	1.00	33.56		0
ATOM			PΑ	28		0.739	30.338	16.131	1.00	36.08		С
ATOM			P A	28		0.038	30.310	17.449	1.00	38.11		С
ATOM		OD1 AS				-0.096	31.392			41.06		0
ATOM	101	OD2 AS	P A	28		-0.392	29.240			41.04		0
MOTA	102	N GL	U A	29		2.737	32.448			32.84		N
ATOM	103		U A			3.288	33.615			31.31		C
ATOM	104		U A			2.792	33.767			29.80		C
MOTA	105		U A			3.547	34.124			29.03		0
MOTA	106		U A			2.938	34.841			31.81		C
MOTA	107		RA			1.524	33.478			28.55		N
MOTA	108		RA			0.957						C C
MOTA	109		RA			1.613				27.25		0
ATOM	110		R A			1.360				26.88 27.71		. C
ATOM	111		RA			-0.546				28.97		0
MOTA	112	OG SE	ER A	. 30		-0.800	32.015	20.320	1.00	20.51		•

											•		
ATOM	113	N	GLN A	. :	31		2.434	31.864	20.994	1.00 26	. 92		N
MOTA	114	CA	GLN A		31		3.089	30.988	21.950	1.00 26	.85		С
MOTA	115	С	GLN A	7	31		4.447	31.558	22.362	1.00 26	6.63		С
MOTA	116	0	GLN A		31		5.115	30.995	23.220	1.00 25	.89		0
MOTA	117	CB	GLN A		31		3.270	29.576	21.375	1.00 26	5.90		С
MOTA	118	CG	GLN A		31	•	1.975	28.816	21.097	1.00 27			С
MOTA	119	CD	GLN A		31		2.227	27.446	20.480	1.00 27			С
ATOM	120		GLN A		31		2.332	27.330	19.262	1.00 28			0
ATOM	121	NE2	GLN A		31		2.354	26.419	21.319	1.00 23			N
ATOM	122	N	LEU A		32		4.835	32.682	21.757	1.00 26			N
ATOM	123	CA	LEU A		32		6.094	33.351	22.078	1.00 26			C
ATOM	124	C	LEU F		32	_	5.854	34.500	23.047	1.00 26			С
ATOM	125	0	LEU A		32		4.875	35.214	22.913	1.00 26			0
ATOM ATOM	126 127	CB CG	LEU A		32 32		6.743 7.054	33.906	20.807	1.00 26			C
ATOM	128		LEU A		32		7.704	32.866 33.537	19.724 18.535	1.00 29			C
ATOM	129		LEU A		32	•	7.942	31.773	20.245		3.07		C
ATOM	130	N	ARG A		33		6.737	34.671	24.026		5.49		Ŋ
ATOM	131	CA	ARG A		33		6.622	35.799	24.957	1.00 26			C
ATOM	132	C	ARG A		33		7.070	37.071	24.252	1.00 26			č
ATOM	133	Ö	ARG A		33		7.810	37.025	23.280	1.00 26			ŏ
ATOM	134	СВ	ARG A		33		7.454	35.554	26.224	1.00 26			Č
ATOM	135	CG	ARG A		33		7.071	34.261	26.976	1.00 25			C
ATOM	136	CD	ARG A		33		7.869	34.029	28.245	1.00 25	5.76		С
MOTA	137	NE	ARG A		33		7.329	32.926	29.021	1.00 25	5.87		N
ATOM	138	CZ	ARG A			-	6.418	33.033	29.969	1.00 25			С
ATOM	139	NHl	ARG A	A	33		5.916	34.198	30.309	1.00 2	4.02		N
MOTA	140	NH2	ARG A	A	33		6.003	31.941	30.587	1.00 28	8.18		N
MOTA	141	N	SER A	A	34		6.643	38.214	24.751	1.00 20	6.73		N
MOTA	142	CA	SER A	A.	34	•	6.939	39.469	24.090	1.00 2	7.21		С
MOTA	143	С	SER A	A	34		8.021	40.251	24.840		6.40		С
MOTA	144	O	SER A		34		7.957	40.391	26.046	1.00 2			0
MOTA	145	CB	SER 2		34		5.657	40.278	24.028	1.00 2			С
MOTA	146	OG	SER I		34		5.402	40.780	25.323	1.00 3			0
ATOM	147	N	TYR		35		9.009	40.750	24.110	1.00 2			N
ATOM	148	CA	TYR .		35		10.169	41.390	24.711	1.00 2			С
ATOM	149	C	TYR .		35		10.412	42.731	24.046	1.00 2			С
MOTA	150	O	TYR .		35		9.815	43.009	23.028	1.00 2		•	0 C
MOTA MOTA	151 152	CB CG.	TYR .		35 35		11.386 11.217	40.479 39.198	24.577 25.357	1.00 2			C
ATOM	153	CD1			35 35		11.041	39.226	26.739	1.00 2			C
ATOM	154		TYR .		35		11.219	37.963	24.723	1.00 2			c
ATOM	155	CE1			35		10.869	38.063	27.459	1.00 2			č
ATOM	156		TYR		35		11.061	36.795	25.445	1.00 2			č
ATOM	157	CZ	TYR		35		10.881	36.847	26.809	1.00 2			Ċ
ATOM	158	ОН	TYR		35		10.698	35.686	27.522	1.00 2			ō
ATOM	159	N	SER		36		11.326	43.531	24.596	1.00 2			N
ATOM	160	CA	SER		36	•	11.555	44.905	24.127	1.00 2			С
ATOM	161	С	SER		36		12.553	45.092	22.987	1.00 2			С
MOTA	162	Ο.	SER		36		12.764	46.211	22.533	1.00 2			0
MOTA	163	CB	SER	Α	36		12.109	45.724	25.286	1.00 2	7.62		С
MOTA	164	OG	SER	A	36		13.365	45.201	25.697	1.00 2	7.53		0
MOTA	165	N	PHE	A	37		13.181	44.025	22.543	1.00 2			N
MOTA	166	CA	PHE		37			44.169	21.590	1.00 2			С
ATOM	167	С	PHE		37		13.949	43.447	20.301	1.00 2			C
MOTA	168	0	PHE		37		13.191	42.512	20.274	1.00 2			0
ATOM	169	CB	PHE		37		15.537	43.571	22.185	1.00 2			С
ATOM	170	CG	PHE		37	•	15.340	42.162	22.731	1.00 2			C
ATOM	171		PHE		37		15.353	41.077	21.890	1.00 2			C
ATOM	172		PHE		37		15:104	41.949	24.076	1.00 2			С
MOTA	173	CEI	. PHE	A	37		15.160	39.778	22.386	1.00 2	2.83		С

ATOM	174	CE2	PHE A		37	14.92	40.		24.578	1.00	22.73			С
MOTA	175	CZ :	PHE A		37	14.94			23.737	1.00				С
ATOM	176	N	PRO A	1	38	14.53			19.222	1.00				N
ATOM	177	CA	PRO A		38	14.39			17.950	1.00				C
ATOM	178	С	PRO A		38	15.32			17.861	1.00				C
ATOM	179	0	PRO P		38	16.28			18.640	1.00				0
ATOM	180	CB	PRO P		38	14.81			16.944	1.00				С
ATOM	181	CG	PRO F	4	38	15.77			17.729	1.00				С
ATOM	182	CD	PRO F	Į.	38	15.27	1 45.	178	19.125		25.73		•	С
ATOM	183	N	THR A	J.	39	15.03			16.902		24.60			N
ATOM	184	CA	THR A	A	39	15.87		979	16.607		24.58			С
ATOM	185	С	THR A	Ą	39	15.88	1 39.	686	15.112		25.39			С
MOTA	186	0	THR A	Ą	39	15.00	4 40.	121	14.383		24.72			0
ATOM.	187	CB	THR A	A	39	15.36		721	17.295		24.33			С
ATOM	188	OG1	THR A	A	39	14.02	3 38.	453	16.860		21.36			0
ATOM	189	CG2	THR A	A	39	15.25		892	18.832		23.91			С
ATOM	190	N	ARG A	A	40	16.87	5 38.	912	14.692		26.09			N
MOTA	191	CA	ARG A	A	40 °	17.00	0 38.	399	13.337		26.92			С
ATOM	192	С	ARG 2	A.	40	17.05	7 36.	884	13.469		26.73	•		С
ATOM	193	0	ARG 2	A.	40	17.40	7 36.	366	14.517		26.53			0
MOTA .	194	CB	ARG :	A	40	18.29	1 38.	888	12.696		27.12			С
MOTA	195	CG	ARG .	A	40	18.28	9 40.	360	12.400		32.37			C
ATOM	196	CD	ARG .	Α	40	16.92	25 40	.858	11.994		36.79		•	С
ATOM	197	NE	ARG	Α	40	16.78	33 41	. 137	10.583		41.20			N
MOTA	198	CZ	ARĠ		40	15.63	L7 41.	. 408	10.023	1.00	46.28			С
ATOM	199	NH1	ARG		40	14.5	12 41	.388	10.768	1.00	47.83			N
ATOM	200		ARG		40	15.5	48 41	.708	8.731	1.00	48.02			N
ATOM	201	N	PRO		41	16.7	28 36	.163	12.413		26.96			N
ATOM	202	CA	PRO		41	16.7	09 34	.706	12.510	1.00	27.17			С
MOTA	203	С	PRO		41	18.0	85 34	.054	12.469		26.50			С
MOTA	204	0	PRO		41	19.0	02 34	.538	11.830	1.00	26.34			0
MOTA	205	CB	PRO		41	15.8	67 34	.277	11.298	1.00	27.12			С
ATOM	206	CG	PRO		41	16.0		.434	10.296	1.00	27.66			С
ATOM	207	CD	PRO		41	16.3		.661	11.077	1.00	26.70			С
ATOM	208	N	ILE		42	18.2	14 32	.951	. 13.185		25.35	•		N
ATOM	209	CA	ILE		42	19.4	00 32	.143	13.070	1.00	24.29			C
ATOM	210	С	ILE		42	19.1	61 31	.290	11.832		23.98			С
ATOM	211	0	ILE		42	18.0	50 30	.793	11.632		24.20			0
MOTA	212	CB	ILE		42	19.5	30 31	.283	14.302	1.00	24.58			С
ATOM	213	CG1			42	19.7	79 32	.181	15.518	1.00	22.71			С
MOTA	214		ILE		42	20.6	44 30	.233	14.113		24.95			С
MOTA	215		ILE		42	19.4	66 31	.516	16.837		22.70			С
ATOM	216		PRO		43	20.1	68 31	.122	10.989		23.44			N
MOTA	217		PRO	A	43	20.0	16 30	.276	9.807		23.74			С
ATOM	218		PRO		43	19.7	09 28	.802	10.154		24.82			С
ATOM	219		PRO		43	20.2		.292	11.130		24.03			0
MOTA	220		PRO	Α	.43	21.3	72 30	.397	9.107		24.23			С
ATOM	221		PRO	Α	43.	22.0	71 31	602	9.740		23.91			C
ATOM	222		PRO	Α	43	21.5	04 31	737	11.092		23.12			С
MOTA	223		ARG	Α	44	18.7	84 28	3.178	9.406		25.20			N
MOTA	224		ARG		44	18.4	39 26	5.767	9.520		26.19			С
MOTA	225		ARG		44	18.9	77 26	5.125	8.269	1.00	25.69			С
ATOM	226		ARG			18.5		5.468	7.159		25.67			0
ATOM	227		ARG			16.9		5.504	9.513		27.16			, C
ATOM	228		ARG			16.3		7.062	10.678		0 31.24			C
ATOM	229		ARG			14.		5.529	10.769		0 32.98			С
ATOM	230		ARG			14.		5.143	10.311		0 34.09			N
ATOM	231		ARG			14.		4.070			0 33.28			С
ATOM	232		1 ARG			14.		4.177			0 29.63			N
ATOM	233		2 ARG			13.	995 2	2.873			0 34.28			N
ATOM	234		LEU			19.		5.174		1.0	0 24.68			N

ATOM	235	CA	LEU	A	45	20.551	24.608	7.302	1.00 24.30	С
ATOM	236	С	LEU	Α	45	20.768	23.134	7.471	1.00 24.39	С
MOTA	237	0	LEU	A	45	20.711	22.623	8.588	1.00 23.97	0
ATOM	238	CB	LEU		45	21.934	25.233	7.205	1.00 23.42	С
ATOM	239	CG	LEU	A	45	21.929	26.724	6.941	1.00 24.95	С
ATOM	240	CD1	LEU	Α	45·	23.339	27.284	7.080	1.00 26.26	С
ATOM	241	CD2	LEU	Α	45	21.375	26.953	5.533	1.00 24.54	. C
ATOM	242	N	SER	Α	46	21.092	22.494	6.352	1.00 24.71	N
ATOM	243	CA	SER		46	21.498	21.119	6.345	1.00 25.24	C
ATOM	244	С	SER		46	22.930	21.043	6.804	1.00 25.58	C
ATOM	245	0	SER		46	23.741	21.908	6.522	1.00 24.65	Ō
ATOM	246	CB	SER		46	21.401	20.505	4.950	1.00 25.11	Ċ
ATOM	247	OG	SER		46	21.863	19.150	4.965	1.00 24.50	ŏ
ATOM	248	N	GLN		47	23.208	19.970	7.517	1.00 26.68	N
ATOM	249	CA	GLN		47	24.524	19.626	8.011	1.00 27.63	c
ATOM	250	C	GLN		47	25.510	19.442	6.853	1.00.28.01	c
ATOM.	251	o	GLN		47	26.704	19.613	7.026	1.00 28.15	Ö
ATOM	252	СВ	GLN		47	24.368	18.317	8.803	1.00 28.89	c
MOTA	253	CG	GLN		47	25.580	17.447	8.920	1.00 20.09	C
ATOM	254	CD	GLN		47	25.826	16.556	7.765	1.00 31.28	C
ATOM	255		GLN		47		•			
ATOM	256					24.906	16.149	7.048	1.00 37.08	0
		NE2			47	27.089	16.213	7.576	1.00 35.81	N
ATOM	257	N	SER		48	25.026	19.086	5.667	1.00 28.11	N
MOTA	258	CA	SER		48	25.930	18.925	4.524	1.00 28.72	C
ATOM	259	C	SER		48	26.222	20.262	3.828	1.00 29.21	C
ATOM	260	0	SER		48	27.068	20.339	2.936	1.00 29.21	. 0
ATOM	261	CB.	SER		48	25.343	17.952	3.508	1.00 28.66	C
MOTA	262	OG	SER		48	24.111	18.440		1.00 29.43	0
ATOM	263	N	ASP		49	25.525	21.314	4.236	1.00 29.60	N
ATOM	264	CA	ASP		49	25.683	22.610	3.596	1.00 30.12	С
MOTA	265	С	ASP		49	26.949	23.307	4.087	1.00 30.43	С
MOTA	266	0	ASP		49	27.100	23.565	5.272	1.00 29.60	0
ATOM	267	CB	ASP	Α	49	24.450	23.458	3.858	1.00 30.26	· C
MOTA	268	CG	ASP		49	24.491	24.792	3.151	1.00 31.74	C
MOTA	269	OD1	ASP	Α	49	25.589	25.306	2.859	1.00 31.79	0
ATOM	270	OD2	ASP	Α	49	23.454	25.418	2.878	1.00 34.13	. 0
ATOM	271	N	PRO	Α	50	27.829	23.668	3.155	1.00 31.31	N
MOTA	272	CA	PRO	A	50	29.123	24.273	3.499	1.00 31.63	С
MOTA	273	С	PRO	Α	50	28.965	25.514	4.355	1.00 31.72	С
MOTA	274	0	PRO	A	50	29.849	25.807	5.164	1.00 31.85	0
ATOM	275	CB	PRO	Α	50	29.726	24.643	2.124	1.00 31.53	С
ATOM	276	CG	PRO		50	29.036	23.738	1.168	1.00 32.13	С
ATOM	277	CD	PRO			27.624	23.620	1.697	1.00 31.55	C
MOTA	278	N	ARG		51	27.875	26.246	4.171	1.00 32.04	N
ATOM	279	CA	ARG			27.648	27.443	4.962	1.00 32.56	C
MOTA	280	С	ARG		51	27.478	27.078	6.439	1.00 32.09	Ċ
MOTA	281	ō	ARG		51	27.853	27.855	7.322	1.00 31.87	o
MOTA	282	СВ	ARG		51	26.420	28.221	4.464	1.00 32.95	C
ATOM	283	CG	ARG		51	26.568	28.810	3.064	1.00 32.33	č
ATOM	284	CD	ARG		51	25.273	29.372	2.480	1.00 34.79	c
ATOM	285	NE			51					N
MOTA	286		ARG			24.276	28.325	2.228	1.00 37.56	
		CZ	ARG		51	22.982	28.564	2.061	1.00 39.54	C
MOTA	287		ARG		51	22.531	29.814	2.124	1.00 40.85	N
MOTA	288		ARG		51	22.135	27.573	1.823	1.00 38.55	N
ATOM	289	N	ALA		52	26.932	25.903	6.721	1.00 31.50	N
. ATOM	290	CA	ALA		52	26.769	25.513	8.117	1.00 31.34	C
ATOM	291	С	ALA		52	28.135	25.310	8.744	1.00 31.24	C
ATOM	292	0	ALA		52	28.409	25.763	9.865	1.00 30.91	0
MOTA	293	CB	ALA		52	25.953	24.284	8.236	1.00 31.35	С
MOTA	294	N	GLU		53	29.005	24.652	8.005	1.00 30.92	N
MOTA	295	ÇA	GLU	A	53	30.332	24.404	8.501	1.00 31.92	С

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ATOM	296 C	: (GLU A	53		31.059	25.730	8.728	1.00 3	31.52		С
ATOM	297 C		GLU A	53		31.766	25.898	9.717	1.00 3	30.52	•	0
ATOM			GLU A	53		31.119	23.554	7.525	1.00 3	32.10		С
			GLU A	53		32.216	22.795	8.229	1.00 3	36.08		С
ATOM						31.776	21.411	8.717	1.00			C
MOTA			GLU A	53				9.167	1.00			Ö
MOTA			GLU A			30.629	21.234					0
MOTA			GLU A			32.606	20.487	8.652	1.00			
ATOM	303 1	N (GLU A	54		30.870	26.665	7.808	1.00			N
MOTA	304	CA (GLU A	54		31.507	27.968	7.919	1.00			С
ATOM		C (GLU A	. 54		31.039	28.685	9.193	1.00	31.07		С
ATOM			GLU A			31.833	29.295	9.881	1.00	31.27		0
ATOM			GLU A			31.218	28.812	6.681	1.00	32.42		С
			GLU A			31.939	30.146	6.669	1.00			С
MOTA							30.966	5.410	1.00			С
ATOM			GLU A			31.662			1.00			Ö
ATOM			GLU A			30.843	30.528	4.558				Ö
MOTA			GLU A			32.268	32.051	5.285	1.00			
ATOM	312	N	LEU A			29.761	28.567	9.534	1.00			N
ATOM	313	CA	LEU A	55	5	29.251	29.240	10.708		28.58		C
ATOM		С	LEU A	55	5	29.848	28.667	11.983		27.91		С
ATOM			LEU F			30.304	29.419	12.841	1.00	26.43		0
ATOM		СВ	LEU A			27.734	29.179	10.733	1.00	28.61		C
		CG	LEU A			27.097	30.041	9.652		28.69		С
ATOM						25.647	29.633	9.423		29.69		С
ATOM			LEU A					10.005		27.60		Ċ
MOTA			LEU A			27.193	31.507			27.51		N
MOTA		N	ILE A			29.889	27.334	12.086				C
MOTA	321	CA	ILE A	A 5	6	30.432	26.679	13.278		27.49		
ATOM	322	С	ILE 2	A 5	6	31.910	27.014	13.457		28.32		C
MOTA	323	0	ILE 2	A 5	6	32.359	27.353	14.549		28.51		0
MOTA		CB	ILE :		6	30.260	25.174	13.192		27.21		С
MOTA	325	CG1				28.771	24.787	13.218	1.00	25.69		С
ATOM	326	CG2			6	30.982	24.505	14.354	1.00	27.65		С
			ILE .		6	28.484	23.341	12.760		23.98		· c
MOTA	327					32.645	26.935	12.357		28.85		N
ATOM	328	N	GLU .		7			12.308		29.98		C
MOTA	329	CA	GLU		7 .	34.068	27.230					Č
MOTA	.330	С	GLU		7	34.319	28.623	12.837		30.12		. 0
ATOM	331	0	GLU		7	35.306	28.869	13.524		31.00	•	
MOTA	332	CB	${ t GLU}$	A 5	7	34.557	27.137	10.850		30.52		C
MOTA	333	CG	GLU	A 5	7	36.003	27.518	10.610	1.00	33.37		С
ATOM	334	CD	GLU	A 5	7	36.968	26.742	11,482	1.00	38.19		С
ATOM	335	OE1			7	36.689	25.558	11.810	1.00	41.02		0
ATOM	336		GLU		7	38.015	27.329	11.847	1.00	42.74		0
	337	N	ASN		8	33.409		12.516		29.57		N
ATOM	338	CA	ASN		8	33.516		12.929	1.00	29.62		С
ATOM						32.852		14.230		27.88		С
ATOM	339	C	ASN		8			14.566		26.74		Ō
MOTA.	340	0	ASN		8	32.690				30.43		č
MOTA	341	CB	ASN .		88	32.805		11.918				c
MOTA	342	CG	ASN		58	33.719		11.040		33.87		
ATOM	343	OD1	ASN	A S	58	34.040	31.918	9.965		36.67		0
MOTA	344	ND2	2 ASN	A !	58	34.189	33.629	11.467		38.66		N
ATOM	345	N	GLU		59	32.396	30.205	14.922		27.73		N
ATOM	346	CA	GLU		59	31.753		16.205	1.00	27.50		С
ATOM	347	C	GLU		59	30.545				26.07		С
	348	0	GLU		59·	30.366				25.28		0
MOTA						32.795				28.12		C
MOTA	349	CB	GLU		59 50					31.06	•	Č
MOTA	350	CG	GLU		59	33.720				35.24		č
MOTA	351	CD	GLU		59	34.739						o
ATOM	352		1 GLU			35.826				39.24		
MOTA	353	OE2	2 GLU	A	59	34.469				37.54		. 0
ATOM	354	N	GLU	A	60	29.691				25.70		N
MOTA	355	CA	GLU	A	60	28.417				25.50		C
MOTA	356	С	GLU		60	27.345	30.576	14.998	1.00	24.10		С

	357	0	GLU	A	60	27.527	29.479	14.487	1.00	22.92	0
TOM	358	СВ	GLU		60	28.402	32.404	13.664	1.00		Č
TOM .	359	CG	GLU		60	29.454	33.497	13.697	1.00		č
MOT	360	CD	GLU	A	60	29.218	34.599	12.703		35.90	Ċ
MOT	361	OE1	GLU		60	29.281	34.349	11.478	1.00		Ō
TOM	362	OE2	GLU	A	60 ·	28.998	35.732	13.165	1.00		Ō
TOM	363	N	PRO		61	26.203	30.933	15.546		22.92	N
TOM	364	CA	PRO		61	25.112	29.983	15.735	1.00		C
TOM	365	С	PRO		61	24.482	29.519	14.445		21.76	Ċ
TOM	366	0	PRO	•	61	24.394	30.252	13.474		21.59	0
TOM	367	CB	PRO	Α	61	24.079	30.775	16.525		22.55	С
TOM	368	CG	PRO	A	61	24.450	32.218	16.380	1.00	21.42	С
MOI	369	CD	PRO	A	61	25.863	32.295	15.967	1.00	22.38	С
IOM	370	N	VAL	Α	62	24.032	28.279	14.444	1.00	21.55	· N
MOI	371	CA	VAL	A	62	23.306	27.739	13.317	1.00	21.90	С
TOM	372	C	VAL		62	22.415	26.622	13.817	1.00	22.38	С
TOM	373	0	VAL		62	22.771	25.886	14.757		22.77	0
TOM	374	CB	VAL		62	24.262	27.217	12.218		22.10	С
MOI	375		VAL		62	25.134	26.112	12.738		22.89	С
TOM	376		VAL		62	23.486	26.748	11.000		21.98	С
TOM	377 ·	N	VAL		63	21.234	26.517	13.226		22.90	N
TOM	378	CA.	VAL		63	20.373	25.398	13.499		23.20	C
TOM	379	C	VAL		63	20.586	24.373	12.378	1.00	23.18	C
MOI MOI	380 381	O CB	VAL		63	20.395	24.682	11.208		23.38	0
MOT	382		VAL VAL		63 63	18.880 18.046	25.768 24.483	13.561 13.754		23.27 24.19	C
MOT	383		VAL		63	18.620		14.692	1.00	22.51	· C
rom	384	N	LEU		64	21.007	23.181	12.756		23.15	N
TOM	385	CA	LEU		64	21.158	22.060	11.835		24.29	C
MO1	386	C	LEU		64	19.904	21.203	11.906		23.48	Č
MOT	387	Ō	LEU		64	19.488	20.816	12.988		23.20	Ö
MO1	388	CB	LEU		64	22.383	21.235	12.206	1.00	24.79	C
FOM	389	CG	LEU	A	64	23.649	22.089	12.141	1.00	28.22	С
MOT	390	CD1	LEU	A	64	24.810	21.338	12.699	1.00	32.80	С
MO1	391	CD2	LEU	Α	64	23.946	22.478	10.719	1.00	30.04	C
MOT	392	N	THR		65	19.308	20.910	10.759	1.00	22.79	· N
rom	393	CA	THR		65	18.019	20.218	10.740	1.00	23.27	С
MO1	394	С	THR		65	18.088	18.730	10.534	1.00	23.05	С
MOI	395	0	THR		65	17.102	18.050	10.765	1.00	22.85	0
MO1	396	CB	THR		65 65	17.150	20.724	9.571	1.00	23.53	C
MO1 MO1	397 398	OG1	THR THR		65 65	17.855	20.496	8.352 9.609		22.75	0
IOM .	399	N.C.GZ	ASP		65 66	16.966 19.231	22.226 18.227			24.78	C
MOJ	400	CA	ASP		66	19.330	16.828	10.093 9.731		23.33 23.76	N C
MOI	401	C	ASP		66	20.581	16.076	10.209		23.70	c
MOI	402	ō	ASP		66	21.117	15.265	9.457		23.64	Ö
MO ¹	403	СВ	ASP		66	19.245	16.732	8.199		23.97	č
MO1	404	CG	ASP		66	20.326	17.517	7.514		24.64	Č
MOJ	405		ASP		66	21.175	18.099	8.223		23.06	ō
MO	406		ASP		66	20.417	17.612	6.268		26.54	. 0
MOJ	407	N	THR	A	67	21.050	16.336	11.428	1.00	22.72	N
MO	408	CA	THR		67	22.235	15.655	11.912	1.00	21.85	C
MO:	409	С	THR		67	21.928	14.246	12.349		21.26	С
MO:	410	0	THR		67	22.813	13.429	12.353		20.41	0
MO.	411	CB	THR		67	22.836	16.345	13.138		21.92	C
MO:	412	OG1			67	21.884	16.347	14.200		20.59	0
MO:	413		THR		67	23.161	17.822	12.873		23.29	C
MO! MO!	414	N	ASN		68 69	20.684	13.993	12.752		20.82	N
.OM !OM	415 416	CA C	ASN ASN		68 68	20.321 21.146	12.741 12.525	13.386 14.652		21.01 20.47	C C
OM!	417	0	ASN		68	21.146	12.323	15.069		20.47	0
. 0.1	71/	0	AON	7	30	21.370	11.3//	13.003	1.00	20.00	O

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MOTA	418		ASN I		68		11.546	12.444	1.00 2			C
MOTA	419		ASN		68	19.476	11.493	11.340	1.00 2			С 0
MOTA	420	OD1			68	18.276	11.429	11.601 10.108	1.00 2			N
ATOM	421	ND2	LEU .		68 69	19.936 21.613	11.492 13.617	15.248	1.00			. N
ATOM	422		LEU . LEU .			22.442	13.533	16.464	1.00			C
ATOM	423		LEU .		69	21.814	12.707.	17.571	1.00			Ċ
ATOM ATOM	424 425		LEU		69	22.492	11.878	18.169	1.00			ō
ATOM	425		LEU		69	22.770	14.907	17.009	1.00			C
ATOM	427		LEU		69	23.654	14.999	18.239	1.00			С
ATOM	428	CD1			69	24.970	14.289	18.035	1.00			·C
ATOM	429	CD2			69	23.911	16.459	18.577	1.00	20.41		С
ATOM	430		VAL		70	20.538	12.940	17.860	1.00	18.84		N
ATOM	431		VAL		70	19.843	12.177	18.894	1.00			С
ATOM	432		VAL		70	18.634 ·	11.447	18.339	1.00	19.17		С
ATOM	433	0	VAL	A	70	17.604	11.325	19.000	1.00	18.71		0
ATOM	434.	CB	VAL	Α	70	19.418	13.038	20.097	1.00		٠	С
ATOM	435	CG1	VAL	A	70	20.645	13.557	20.812	1.00			С
ATOM	436	CG2	VAL	A	70	18.513	14.185	19.686		18.87		С
MOTA	437	N	TYR	Α	71	18.796	10.916	17.133		20.12		N
MOTA	438	CA	TYR	A	71	17.711	10.224	16.454		20.64		C
ATOM	439	С	TYR		71	17.003	9.218	17.377		20.76		C
MOTA	440	0	TYR		71	15.804	9.275	17.507		20.54		0
MOTA	441	CB	TYR		71	18.186	9.591	15.136		20.75		C
MOTA	442	CG	TYR		71	17.243	8.517	14.628		23.02		C
MOTA	443	CD1			71	16.012	8.837	14.046		24.62		C
MOTA	444	CD2	TYR		71	17.572	7.182	14.754		22.94 23.64		C
ATOM	445	CE1	TYR		71	15.132	7.800	13.595 14.312		23.48		C
ATOM	446	CE2	TYR		71	16.730	6.174 6.478	13.730		24.03		C
ATOM	447	CZ	TYR		71	15.524	5.422	13.730		29.55		ŏ
MOTA	448	OH	TYR		71	14.697 17.728	8.356	18.068		21.35		Ŋ
ATOM	449 450	N CA	PRO PRO		72 72	17.720	7.363	18.945		21.89		Č
MOTA MOTA	451	C	PRO		72	16.296	7.955	20.106		22.22		С
ATOM	452	Ö	PRO		72	15.432	7.269	20.628		21.25		0
ATOM	453	СВ	PRO		72	18.248	6.538	19.493		21.83		C
ATOM	454	CG	PRO		72	19.420	6.849	18.606		22.53		. C
MOTA	455	CD	PRO		72	19.192	8.240	18.080	1.00	21.81		С
ATOM	456	N	ALA		73	16.568	9.206	20.484	1.00	22.77		N
ATOM	457	CA	ALA	A	73	15.859	9.836	21.605	1.00	23.23		С
MOTA	458	Ċ	ALA	A	73	14.542	10.487	21.178	-	23.64		С
MOTA	459	0	ALĀ	A	73	13.764	10.966			23.47		0
MOTA	460	СВ	ALA	Α	73	16.750	10.860			22.77		С
MOTA	461	N	LEU	JA	74	14.275	10.507			24.25		N
MOTA	462	CA	LEU		74	13.057	11.148			24.86		С
MOTA	463	С	LEU		74	11.792	10.466			25.46		C
MOTA	464	0	LEU		74	10.729	11.070			25.11		0
MOTA	465		LEU		74	13.055	11.240			24.77		C
ATOM	466		LEC		74	14.160				26.74		C
MOTA	467		LEU		74	13.915				26.86		C
ATOM	468		LEC		74	14.288	13.447			26.12		N
ATOM	469			5 A		11.908 10.756				26.39		C
MOTA	470			S A S A		10.736				26.71		.c
MOTA	471			S A		9.584				26.80		0
ATOM ATOM	472 473			S A		10.918				26.36		Č
ATOM	474			SA		12.141				26.49		Ċ
MOTA	475			S A		12.254				27.59		C
MOTA	476			SA		13.732				27.21		C
MOTA	477			SA		14.475				24.71		N
MOTA	478			P A		11.561				26.64		N
111 011	3,0			- ••	•							

ATOM ·	479	CA	TRP 2		76	11.484	9.557	24.383	1.00 26	.78	С
MOTA	480	С	TRP I		76	10.253	10.368	24.770	1.00 27		С
ATOM	481	0	TRP 2		76	9.889	11.317	24.095	1.00 27		0
MOTA	482	CB	TRP :		76	12.717	10.311	24.888	1.00 26		C
ATOM	483	CG	TRP :		76	13.963	9.500	24.895	1.00 25		С
ATOM	484	CD1			76	14.101	8.219	24.486	1.00 24		С
MOTA	485	CD2	TRP .		76 76	15.255	9.917	.25.347	1.00 22		С
ATOM ATOM	486 487	NE1 CE2	TRP .		76 76	15.399	7.804	24.647	1.00 23		N
ATOM	488	CE3	TRP		76 76	16.128 15.767	8.829 11.107	25.178	1.00 22		С
ATOM	489	CZ2			76	17.468	8.890	25.867 25.520	1.00 21 1.00 22		C C
ATOM ·	490	CZ3	TRP		76	17.090	11.172	26.202	1.00 22		C
ATOM	491	CH2			76	17.931	10.076	26.029		.36	C
ATOM	492	N	ASP		77	9.639	9.976	25.880	1.00 27		N
ATOM	493	CA	ASP		77	8.532	10.684	26.484	1.00 27		Ĉ
MOTA	494	С	ASP		77	8.560	10.277	27.957	1.00 27		Ċ
MOTA	495	0	ASP	A	77	9.373	9.460	28.336	1.00 27		0
MOTA	496	CB	ASP	Α	77	7.208	10.368	25.800		.89	С
MOTA	497	CG	ASP		77	6.802	8.913	25.903	1.00 29	.06	С
MOTA	498		ASP		77	7.354	8.108	26.708	1.00 30	.51	0
MOTA	499		ASP		77	5.894		·25.179·		13	0
ATOM	500	N	LEU		78	7.710	10.847	28.796	1.00 27		N
ATOM	501	CA	LEU		78	7.819	10.578	30.229.			C
ATOM	502	C	LEU		78	7.655	9.101	30.542	1.00 27		C
MOTA MOTA	503 504	·O CB	LEU LEU		78 70	8.386	8.548	31.367	1.00 27	-	0
ATOM	505	.CG	LEU		78 78	6.818	11.409 12.916	31.011		7.59	C
ATOM	506		LEU		78	7.007 5.906	13.677	30.880 31.612	1.00 28 1.00 28	68	C C
ATOM	507		LEU		78	8.369	13.328	31.412		9.32	C
ATOM	508	N	GLU		79	6.721	8.450	29.860		3.17	N
ATOM	509	CA	GLU		79	6.480	7.035	30.102		3.56	C
ATOM	510	С	GĿŪ		79	7.715	6.185	29.781	1.00 28		Ċ
ATOM	511	0	GLU		79	8.167	5.388	30.600	1.00 27		Ō
ATOM	512	CB	GLU	A	79	5.267	6.540	29.298	1.00.28		С
ATOM '	513	CG	GLU	A	79	5.051	5.049	29.467	1.00 31		C
MOTA	514	CD	GLU		79	3.849	4.516	28.716		1.79	С
MOTA	515	OE1	-		79	3.422	5.129	27.709		5.78	0
ATOM	516		GLU		79	3.343	3.457	29.144		7.92	0
ATOM	517	N	TYR.		80	8.260	6.346	28.582		3.27	N
ATOM · ATOM	518 519	CA C	TYR		80 -	9.452	5.597	28.200	1.00 28		C
ATOM	520	0	TYR		80 80	10.628	5.873	29.142	1.00 27 1.00 27		С
ATOM	521	СВ	TYR TYR		80	11.330 9.838	4.958 5.964	29.563 26.787	1.00 28		0
ATOM	522	CG	TYR		80	11.054	5.250	26.787	1.00 27		C
MOTA	523		TYR		80	10.952	3.991	25.644	1.00 27		C
ATOM	524		TYR		80	12.300	5.846	26.306	1.00 25		č
MOTA	525		TYR		80	12.089	3.352	25.128	1.00 26		Ċ
MOTA	526		TYR		80	13.417	5.224	25.808	1.00 25		·C
MOTA	527	CZ	TYR		80 .	. 13.320	3.992	25.213	1.00 25		C
ATOM	528	ОН	TYR	Α	80	14.467	3.426	24.703	1.00 23	3.50	0
ATOM	529	N	LEU		81	10.839	7.135	29.482	1.00 27		N
MOTA	530	CA	LEU		81	11.952	7.477	30.371	1.00 27		С
ATOM	531	C	LEU		81	11.741	6.943	31.801	1.00 27		С
MOTA	532	0	LEU		81	12.682	6.459	32.437	1.00 27		0
MOTA	533	CB	LEU		81	12.194	8.990	30.399	1.00 27		C
MOTA MOTA	534 535	CG	LEU		81	12.659	9.656	29.096	1.00 28		C
ATOM	536		LEU LEU		81 81	12.664 14.036	11.170 9.192	29.269	1.00 28		C
ATOM	537	N	GLN		8.2	10.521	7.049	28.655 32.313	1.00 27		C
ATOM	538	CA	GLN		82	10.234	6.557	33.656	1.00 28		N C
ATOM	539	C	GLN		82	10.525	5.066	33.689	1.00 28		C
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MOTA	540 O GLN A 82				1.00 28.25
MOTA	541 CB GLN A 82	8.774 6.			L.00 29.04
ATOM	542 CG GLN A 82	8.325 6.			1.00 30.18
ATOM	543 CD GLN A 82	7.184 6.			1.00 32.25
ATOM	544 OE1 GLN A 82	6.642 7	.758 35		1.00 34.51
ATOM	545 NE2 GLN A. 82	6.822 6	.204 37	7.189	1.00 36.79
	546 N GLU A 83				1.00 28.58
ATOM	547 CA GLU A 83				1.00 28.70
ATOM					1.00 28.14.
ATOM					1.00 27.54
ATOM	549 O GLU A 83				1.00 28.53
MOTA	550 CB GLU A 83				1.00 20.33
MOTA	551 CG GLU A 83				1.00 33.70
ATOM	552 CD GLU A 83				1.00 35.31
MOTA	553 OE1 GLU A 83				1.00 35.22
MOTA	554 OE2 GLU A 83				
ATOM	555 N ASNA 84				1.00 27.44
MOTA	556 CA ASN A 84			1.400	1.00 27.09
ATOM	557 C ASN A 84			1.913	1.00 27.31
MOTA	558 O ASN A 84			1.759	1.00 27.17
ATOM	559 CB ASN A 84			9.879	1.00.27.17
ATOM	560 CG ASN A 84	13.226 1	1.890 2	9.254	1.00 26.24
ATOM	561 OD1 ASN A 84	13.361	.696 2	9.532	1.00 27.49
ATOM	562 ND2 ASN A 84 .		2.333 2	8.413	1.00 23.37
ATOM	563 N ILE A 85			32.511	1.00 27.52
	564 CA ILE A 85			32.861	1.00 28.25
MOTA	565 C ILE A 85			34.185	1.00 28.03
MOTA				34.610	1.00 28.40
ATOM				32.801	1.00 28.23
MOTA				32.342	1.00 29.61
MOTA	568 CG1 ILE A 85			34.139	1.00 29.11
ATOM	569 CG2 ILE A 85			31.996	1.00 28.97
MOTA	570 CD1 ILE A 85				1.00 28.14
MOTA	571 N GLY A 86			34.833	1.00 28.14
MOTA	.572 CA GLY A 86			36.061	1.00 28.11
MOTA	573 C GLY A 86			37.335	
MOTA	574 O GLY A 86			37.308	1.00 27.93
MOTA	575 N ASNA 87			38.444	1.00 27.96
MOTA	576 CA ASN A 87			39.767	1.00 27.88
MOTA	577 C ASN A 87			40.373	1.00 27.82
MOTA	578 O ASN A 87			41.585	1.00 27.63
ATOM	579 CB ASN A 87	16.571		40.713	1.00 27.89
MOTA	580 N GLY A 88	18.559		39.538	1.00 28.21
ATOM	581 CA GLY A 88	19.478		40.006	1.00 28.18
ATOM	582 C GLY A 88	18.706	8.584	40.396	1.00 28.19
ATOM	583 O GLY A 88	17.520	8.676	40.097	1.00 28.62
ATOM	584 N ASP A 89	19.357	9.530	41.068	1.00 27.99
ATOM	585 CA ASP A 89		10.781	41.468	1.00 28.09
ATOM	586 C ASP A 89		11.806	40.335	1.00 28.00
ATOM	587 O ASP A 89		11.866	39.507	1.00 28.07
ATOM	588 CB ASP A 89		11.433	42.613	1.00 28.24
	589 CG ASP A 89		10.747	43.935	1.00 28.53
ATOM		18.398	9.843	44.024	1.00 30.26
MOTA			11.070	44.955	1.00 29.31
MOTA			12.637	40.330	1.00 27.56
ATOM	592 N PHE A 90		13.687	39.332	1.00 27.37
MOTA	593 CA PHE A 90		15.037	39.993	1.00 27.78
ATOM	594 C PHE A 90		15.171	40.884	1.00 27.70
ATOM	595 O PHE A 90		13.388	38.351	1.00 27.05
MOTA					1.00 27.05
MOTA	597 CG PHE A 90		12.262	37.408	
MOTA	598 CD1 PHE A 90		10.943	37.806	
MOTA	599 CD2 PHE A 90		12.521	36.121	
ATOM	600 CE1 PHE A 90	16.797	9.908	36.943	1.00 24.06

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ATOM .	601	CE2	PHE A	90	17.395	11.489	35.248	1.00 25.49	С
ATOM	602		PHE A		17.235	10.176	35.666	1.00 25.33	С
MOTA	603	N	SER A		18.062	16.033	39.560	1.00 27.85	N
MOTA	604	CA	SER A		17.902	17.384	40.075	1.00 28.17	С
ATOM	605	С	SER F		16.695	18.023	39.419	1.00 28.48	C
ATOM	606	0	SER A		16.589	18.085	38.192	1.00 28.35	0
ATOM	607		SER F		19.149	18.236	39.838	1.00 27.86	C
ATOM	608	OG	SER A		20.260	17.652	40.485	1.00 27.15	0
ATOM	609	N	VAL A		15.784	18.482	40.261	1.00 29.05	N
ATOM .	610	CA	VAL A		14.585	19.141 20.465	39.812 40.529	1.00 29.67 1.00 30.31	C C
ATOM ATOM	611 612	C 0	VAL A		14.437 14.442	20.465	41.763	1.00 30.31	0
ATOM	613	CB	VAL A		13.352	18.313	40.106	1.00 30.37	C
ATOM	614		VAL A		12.106	19.026	39.582	1.00 29.93	C
ATOM	615		VAL A		13.490	16.930	39.507	1.00 29.60	Č
ATOM	616	N	TYR A		14.329	21.516	39.732	1.00 31.00	N
ATOM	617	CA	TYR A		14.135	22.845	40.241	1.00 31.29	Ċ
MOTA	618	C	TYR A		12.662	23.113	40.298	1.00 31.54	Č
MOTA	619	Ö	TYR A		11.892	22.701	39.423	1.00 31.35	0
ATOM	620	CB.			. 14.829	23.853	39.345	1.00 31.87	C
ATOM	621	CG	TYR A		16.310	23.711	39.436	1.00 33.05	С
ATOM	622	CD1	TYR Z		. 17.012	24.283	40.482	1.00 34.67	С
ATOM	.623	CD2	TYR Z	A 93	16.998	22.954	38.525	1.00 34.24	С
ATOM	624	CE1	TYR A	A 93	18.357	24.125	40.593	1.00 35.09	С
ATOM	625	CE2	TYR Z	A 93	18.338	22.789	38.634	1.00 36.36	С
MOTA	626	CZ	TYR .		19.011	23.379	39.670	1.00 36.33	С
ATOM	627	ОН	TYR 2		20.357	23.204	39.772	1.00 40.81	0
ATOM	628	N	SER		12.286	·23.813	41.351	1.00 32.03	N
ATOM .	629	CA	SER		10.919	24.182	41.599	1.00 32.31	С
ATOM	630	С	SER .		10.884	25.692	41.704	1.00 32.42	. C
ATOM	631	0	SER .		11.743	26.286		1.00 32.48	0
ATOM	632	СВ	SER .		10.464		42.914	1.00 32.38	C
ATOM	633	OG	SER .		9.062	23.691	43.052	1.00 33.53	0
ATOM	634	N	ALA		9.902	26.314	41.070	1.00 32.58	N
ATOM	635	CA	ALA		9.766	27.757	41.135	1.00 32.90	C
ATOM	636 637	C	ALA		8.312 7.446	28.172	41.076 40.620	1.00 33.48 1.00 33.62	0
MOTA MOTA	638	СВ	ALA ALA			27.429 28.413	39.996	1.00 33.02	C
ATOM	639	И	SER			29.382	41.539	1.00 32.00	N
ATOM	640 [°]	CA	SER			29.932	41.482	1.00 34.75	C
ATOM	641	C	SER			30.974	40.382	1.00 34.75	č
ATOM	642	ŏ	SER			31.659	40.275	1.00 35.29	ő
ATOM	643	СВ	SER			30.592	42.801	1.00 35.05	c
ATOM	644	OG	SER			31.311	42.627	1.00 36.18	ō
ATOM	645	N	THR			31.107	39.593	1.00 33.88	N
ATOM	646	CA	THR			32.046	38.477	1.00 33.41	С
ATOM	647	C	THR			31.238	37.265	1.00 32.32	С
ATOM	648	0	THR			30.143	37.411	1.00 32.10	0
ATOM	649	CB	THR		8.797	33.144	38.695	1.00 33.64	C
MOTA	650		THR			33.810	37.460	1.00 33.76	0
MOTA	651	CG2	THR	A 97	10.190	32.559	39.058	1.00 34.25	С
ATOM	652	N	HIS	A 98	7.840	31.762	36.073	1.00 31.47	N
MOTA	653	CA	HIS	A 98	8.278	31.071	34.863	1.00 30.97	C
MOTA	654	С	HIS			31.134	34.707	1.00 30.53 ⁻	С
ATOM	655	0	HIS			30.379	33.940	1.00 29.14	0
ATOM	656	CB	HIS				33.621	1.00 31.14	C
ATOM	657	CG	HIS			33.125	33.415	1.00 30.86	С
ATOM	658		HIS			34.112	34.011	1.00 31.51	· N
ATOM	659		HIS				32.651	1.00 31.48	C
MOTA	660		HIS				33.634	1.00 31.14	C
MOTA	661	NE2	HIS	A 98	8.581	35.118	32.805	1.00 30.50	N

ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	662 663 664 665 666 667	N CA C	LYS			10 450	20 22-	05		
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	664 665 666				99	10.459	32.025	35.449	1.00 30.36	N
ATOM ATOM ATOM ATOM ATOM ATOM	665 666	С	LYS	A	99	11.895	32.198	35.298	1.00 31.07	С
ATOM ATOM ATOM ATOM ATOM	665 666		LYS .	Α	99	12.761	31.288	36.166	1.00 31.00	
ATOM ATOM ATOM ATOM ATOM	666	0	LYS		99	12.693				
ATOM ATOM ATOM ATOM ATOM							31.337	37.396	1.00 31.91	
ATOM ATOM ATOM ATOM	667	CB	LYS .		99	12.265	33.643	35.544	1.00 31.15	С
ATOM ATOM ATOM		CG	LYS .	Α·	99	11.887	34.551	34.391	1.00 33.39	C
ATOM ATOM ATOM	668	CD	LYS .	Α	99	12.486	35.945	34.556	1.00 36.16	
ATOM ATOM	669	CE	LYS		99					_
MOTA						11.763	36.771	35.607	1.00 37.52	С
	670	NZ	LYS .		99	10.620	37.507	35.006	1.00 38.84	N
A TOM	671	N	PHE .	A :	100	13.572	30.453	35.518	1.00 30.20	
MION	672	CA	PHE .	A :	100	14.517	29.606	36.232	1.00 30.03	= -
MOTA	673	C	PHE							_
						15.952	30.123	36.138	1.00 29.72	С
MOTA	674	0	PHE .			16.826	29.544	35.481	1.00 29.39	. 0
MOTA	675	CB	PHE .	A :	100	14.441	28.168	35.744	1.00 29.93	
ATOM	676	·CG	PHE .			13.223	27.452	36.206		
ATOM	677		PHE						1.00 29.72	
						12.014	27.637	35.566	1.00 28.98	С
ATOM	678		PHE .			13.283	26.596	37.289	1.00 30.77	С
MOTA	679	CE1	PHE .	A :	100	10.896	26.969	35.983	1.00 30.22	С
MOTA	680	CE2	PHE .	A :	100	12.158	25.919	37.719	1.00 30.51	
ATOM	681	CZ	PHE							С
						10.967	26.105	37.069	1.00 30.63	C
MOTA	682	N	LEU .			16.178	31.235	36.809	1.00 29.87	N
ATOM	683	CA	LEU .	Α:	101 ·	17.495	31.812	36.919	1.00 29.57	C
ATOM	684	С	LEU .			18.451	30.814	37.555	1.00 29.61	
ATOM	685	0	LEU							С
						18.249	30.380	38.679	1.00 28.35	0
ATOM	686	CB	LEU .			17.412	33.057	37.787	1.00 29.68	С
ATOM	687	CG	LEU .	A :	101 ·	18.707	33.845	37.954	1.00 29.68	С
ATOM	688	CD1	LEU .	A :	101	19.184	34.337	36.620	1.00 28.70	
MOTA	689	CD2	LEU .			18.474				
							35.014	38.909	1.00 31.41	C
ATOM	690	N	TYR .			19.490	30.440	36.816	1.00 30.36	. И
MOTA	691	CA	TYR .	A :	102	20.516	29.535	37.338	1.00 30.64	С
ATOM	692	C	TYR .	A :	102	21.332	30.228	38.440	1.00 30.93	
ATOM	693	0	TYR							
						21.623	31.425	38.339	1.00 30.67	0
ATOM	.694	CB	TYR .			21.480	29.101	36.224	1.00 30.45	С
MOTA	695	CG	TYR .	A :	102	22.609	28.271	36.774	1.00 31.25	C
ATOM	696	CD1	TYR .	A :	102	22.430	26.916	37.062	1.00 31.33	Č
ATOM	697		TYR							
ATOM	698					23.842	28.844	37.054	1.00 31.29	
			.TYR			23.456	26.163	37.612	1.00 32.81	С
MOTA	699	CE2	TYR .	A :	102	24.869	28.098	37.601	1.00 32.24	С
MOTA	700	CZ	TYR :	A :	102	24.676	26.764	37.876	1.00 34.18	c
MOTA	701	ОН	TYR			25.720				
ATOM	702						26.030	38.418	1.00 39.06	0
		N	TYR .			21.684	29.478	39.488	1.00 31.28	N
MOTA	703	CA	TYR :	A 3	103	22.569	29.983	40.539	1.00 31.56	
MOTA	704	С	TYR 3	A :	103 .	23.524				
TION							20.911	41.058		•
		0	TYR :	a 1	เกร		28.911	41.058	1.00 31.11	·c
MOTA	705	O CB	TYR			23.190	27.732	41.165	1.00 31.11 1.00 30.75	· C
ATOM ATOM	705 706	CB	TYR :	A 1	103	23.190 21.796	27.732 30.599		1.00 31.11	· C
ATOM ATOM ATOM	705 706 707	CB CG	TYR I	A 1 A 1	103 103	23.190	27.732	41.165 41.706	1.00 31.11 1.00 30.75 1.00 31.98	. o
ATOM ATOM	705 706	CB CG	TYR I	A 1 A 1	103 103	23.190 21.796 20.846	27.732 30.599 29.663	41.165 41.706 42.385	1.00 31.11 1.00 30.75 1.00 31.98 1.00 33.92	0000
MOTA MOTA MOTA	705 706 707 708	CB CG CD1	TYR I	A 1 A 1 A 1	103 103 103	23.190 21.796 20.846 19.577	27.732 30.599 29.663 29.445	41.165 41.706 42.385 41.868	1.00 31.11 1.00 30.75 1.00 31.98 1.00 33.92 1.00 36.08	00000
MOTA MOTA MOTA MOTA	705 706 707 708 709	CB CG CD1 CD2	TYR Z TYR Z TYR Z TYR Z	A 1 A 1 A 1 A 1	103 103 103 103	23.190 21.796 20.846 19.577 21.203	27.732 30.599 29.663 29.445 29.010	41.165 41.706 42.385 41.868 43.553	1.00 31.11 1.00 30.75 1.00 31.98 1.00 33.92 1.00 36.08 1.00 36.91	000000
ATOM ATOM ATOM ATOM ATOM	705 706 707 708 709 710	CB CG CD1 CD2 CE1	TYR 7 TYR 7 TYR 7 TYR 7 TYR 7	A 1 A 1 A 1 A 1	103 103 103 103 103	23.190 21.796 20.846 19.577 21.203 18.696	27.732 30.599 29.663 29.445	41.165 41.706 42.385 41.868	1.00 31.11 1.00 30.75 1.00 31.98 1.00 33.92 1.00 36.08	000000
ATOM ATOM ATOM ATOM ATOM ATOM	705 706 707 708 709 710 711	CB CG CD1 CD2 CE1 CE2	TYR 7 TYR 7 TYR 7 TYR 7 TYR 7 TYR 7	A 1 A 1 A 1 A 1 A 1	103 103 103 103 103 103	23.190 21.796 20.846 19.577 21.203	27.732 30.599 29.663 29.445 29.010	41.165 41.706 42.385 41.868 43.553 42.483	1.00 31.11 1.00 30.75 1.00 31.98 1.00 33.92 1.00 36.08 1.00 36.91 1.00 37.42	00000000
ATOM ATOM ATOM ATOM ATOM	705 706 707 708 709 710	CB CG CD1 CD2 CE1	TYR 7 TYR 7 TYR 7 TYR 7 TYR 7 TYR 7	A 1 A 1 A 1 A 1 A 1	103 103 103 103 103 103	23.190 21.796 20.846 19.577 21.203 18.696 20.325	27.732 30.599 29.663 29.445 29.010 28.587 28.153	41.165 41.706 42.385 41.868 43.553 42.483 44.189	1.00 31.11 1.00 30.75 1.00 31.98 1.00 33.92 1.00 36.08 1.00 36.91 1.00 37.42 1.00 37.63	000000000
ATOM ATOM ATOM ATOM ATOM ATOM ATOM	705 706 707 708 709 710 711 712	CB CG CD1 CD2 CE1 CE2	TYR 7 TYR 7 TYR 7 TYR 7 TYR 7 TYR 7 TYR 7	A 1 A 1 A 1 A 1 A 1 A 1	103 103 103 103 103 103 103	23.190 21.796 20.846 19.577 21.203 18.696 20.325 19.070	27.732 30.599 29.663 29.445 29.010 28.587 28.153 27.947	41.165 41.706 42.385 41.868 43.553 42.483 44.189 43.647	1.00 31.11 1.00 30.75 1.00 31.98 1.00 33.92 1.00 36.08 1.00 36.91 1.00 37.42 1.00 37.63 1.00 38.74	0000000000
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	705 706 707 708 709 710 711 712 713	CB CG CD1 CD2 CE1 CE2 CZ OH	TYR 7 TYR 7 TYR 7 TYR 7 TYR 7 TYR 7 TYR 7 TYR 7	A 1 A 1 A 1 A 1 A 1 A 1	103 103 103 103 103 103 103	23.190 21.796 20.846 19.577 21.203 18.696 20.325 19.070 18.183	27.732 30.599 29.663 29.445 29.010 28.587 28.153 27.947 27.099	41.165 41.706 42.385 41.868 43.553 42.483 44.189 43.647 44.264	1.00 31.11 1.00 30.75 1.00 31.98 1.00 36.08 1.00 36.91 1.00 37.42 1.00 37.63 1.00 38.74 1.00 40.90	00000000000
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	705 706 707 708 709 710 711 712 713 714	CB CG CD1 CD2 CE1 CE2 CZ OH N	TYR 7 TYR 7 TYR 7 TYR 7 TYR 7 TYR 7 TYR 7 TYR 7 TYR 7 TYR 7	A 1 A 1 A 1 A 1 A 1 A 1	103 103 103 103 103 103 103 103	23.190 21.796 20.846 19.577 21.203 18.696 20.325 19.070 18.183 24.725	27.732 30.599 29.663 29.445 29.010 28.587 28.153 27.947 27.099 29.345	41.165 41.706 42.385 41.868 43.553 42.483 44.189 43.647 44.264 41.391	1.00 31.11 1.00 30.75 1.00 31.98 1.00 36.08 1.00 36.91 1.00 37.42 1.00 37.63 1.00 38.74 1.00 40.90 1.00 30.34	00000000000
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	705 706 707 708 709 710 711 712 713 714 715	CB CG CD1 CD2 CE1 CE2 CZ OH N	TYR I TYR I	A 1 A 1 A 1 A 1 A 1 A 1 A 1	103 103 103 103 103 103 103 103 104	23.190 21.796 20.846 19.577 21.203 18.696 20.325 19.070 18.183	27.732 30.599 29.663 29.445 29.010 28.587 28.153 27.947 27.099 29.345	41.165 41.706 42.385 41.868 43.553 42.483 44.189 43.647 44.264	1.00 31.11 1.00 30.75 1.00 31.98 1.00 36.08 1.00 36.91 1.00 37.42 1.00 37.63 1.00 38.74 1.00 40.90 1.00 30.34	000000000000000000000000000000000000000
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	705 706 707 708 709 710 711 712 713 714	CB CG CD1 CD2 CE1 CE2 CZ OH N	TYR I TYR I	A 1 A 1 A 1 A 1 A 1 A 1 A 1	103 103 103 103 103 103 103 103 104	23.190 21.796 20.846 19.577 21.203 18.696 20.325 19.070 18.183 24.725 25.752	27.732 30.599 29.663 29.445 29.010 28.587 28.153 27.947 27.099 29.345 28.444	41.165 41.706 42.385 41.868 43.553 42.483 44.189 43.647 44.264 41.391 41.873	1.00 31.11 1.00 30.75 1.00 31.98 1.00 36.08 1.00 36.91 1.00 37.42 1.00 37.63 1.00 38.74 1.00 40.90 1.00 30.34 1.00 30.04	000000000000000000000000000000000000000
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	705 706 707 708 709 710 711 712 713 714 715 716	CB CG CD1 CD2 CE1 CE2 CZ OH N CA C	TYR TYR TYR TYR TYR TYR TYR TYR TYR ASP ASP ASP	A 1 A 1 A 1 A 1 A 1 A 1 A 1	103 103 103 103 103 103 103 104 104	23.190 21.796 20.846 19.577 21.203 18.696 20.325 19.070 18.183 24.725 25.752 25.735	27.732 30.599 29.663 29.445 29.010 28.587 28.153 27.947 27.099 29.345 28.444 28.408	41.165 41.706 42.385 41.868 43.553 42.483 44.189 43.647 44.264 41.391 41.873 43.394	1.00 31.11 1.00 30.75 1.00 31.98 1.00 36.08 1.00 36.91 1.00 37.42 1.00 37.63 1.00 38.74 1.00 40.90 1.00 30.34 1.00 30.04 1.00 29.73	000000000000000000000000000000000000000
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	705 706 707 708 709 710 711 712 713 714 715 716 717	CB CG CD1 CD2 CE1 CE2 CZ OH N CA C	TYR TYR TYR TYR TYR TYR TYR TYR TYR TYR	A 1 A 1 A 1 A 1 A 1 A 1 A 1 A 1 A 1 A 1	103 103 103 103 103 103 103 104 104 104	23.190 21.796 20.846 19.577 21.203 18.696 20.325 19.070 18.183 24.725 25.752 25.752 26.079	27.732 30.599 29.663 29.445 29.010 28.587 28.153 27.947 27.099 29.345 28.444 28.408 29.388	41.165 41.706 42.385 41.868 43.553 42.483 44.189 43.647 44.264 41.391 41.873 43.394 44.062	1.00 31.11 1.00 30.75 1.00 31.98 1.00 36.08 1.00 36.91 1.00 37.42 1.00 37.63 1.00 38.74 1.00 40.90 1.00 30.34 1.00 30.04 1.00 29.73 1.00 28.53	000000000000000000000000000000000000000
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	705 706 707 708 709 710 711 712 713 714 715 716 717	CB CG CD1 CD2 CE1 CE2 CZ OH N CA C O	TYR TYR TYR TYR TYR TYR TYR TYR TYR ASP ASP ASP ASP ASP ASP	A 11 A 11 A 11 A 11 A 11 A 11 A 11	103 103 103 103 103 103 103 104 104 104	23.190 21.796 20.846 19.577 21.203 18.696 20.325 19.070 18.183 24.725 25.752 25.752 26.079 27.089	27.732 30.599 29.663 29.445 29.010 28.587 28.153 27.947 27.099 29.345 28.444 28.408 29.388 28.931	41.165 41.706 42.385 41.868 43.553 42.483 44.189 43.647 44.264 41.391 41.873 43.394 44.062 41.350	1.00 31.11 1.00 30.75 1.00 31.98 1.00 36.08 1.00 36.91 1.00 37.42 1.00 37.63 1.00 38.74 1.00 40.90 1.00 30.34 1.00 30.04 1.00 29.73 1.00 28.53 1.00 30.07	000000000000000000000000000000000000000
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	705 706 707 708 709 710 711 712 713 714 715 716 717 718 719	CB CG CD1 CD2 CE1 CE2 CZ OH N CA C O CB	TYR TYR TYR TYR TYR TYR TYR TYR TYR ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	A 11 A A 11 A A A 11 A A A 11 A A A 11 A A A 11	103 103 103 103 103 103 103 104 104 104 104	23.190 21.796 20.846 19.577 21.203 18.696 20.325 19.070 18.183 24.725 25.752 25.752 26.079	27.732 30.599 29.663 29.445 29.010 28.587 28.153 27.947 27.099 29.345 28.444 28.408 29.388	41.165 41.706 42.385 41.868 43.553 42.483 44.189 43.647 44.264 41.391 41.873 43.394 44.062 41.350	1.00 31.11 1.00 30.75 1.00 31.98 1.00 36.08 1.00 36.91 1.00 37.42 1.00 37.63 1.00 38.74 1.00 40.90 1.00 30.34 1.00 30.04 1.00 29.73 1.00 28.53 1.00 30.07	000000000000000000000000000000000000000
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	705 706 707 708 709 710 711 712 713 714 715 716 717	CB CG CD1 CD2 CE1 CE2 CZ OH N CA C O CB	TYR TYR TYR TYR TYR TYR TYR TYR TYR ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	A 11 A A 11 A A A 11 A A A 11 A A A 11 A A A 11	103 103 103 103 103 103 103 104 104 104 104	23.190 21.796 20.846 19.577 21.203 18.696 20.325 19.070 18.183 24.725 25.752 25.735 26.079 27.089 28.233	27.732 30.599 29.663 29.445 29.010 28.587 28.153 27.947 27.099 29.345 28.444 28.408 29.388 28.931 28.037	41.165 41.706 42.385 41.868 43.553 42.483 44.189 43.647 44.264 41.391 41.873 43.394 44.062 41.350 41.731	1.00 31.11 1.00 30.75 1.00 31.98 1.00 36.08 1.00 36.91 1.00 37.42 1.00 37.63 1.00 38.74 1.00 40.90 1.00 30.34 1.00 29.73 1.00 28.53 1.00 30.07 1.00 30.02	000000000000000000000000000000000000000
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	705 706 707 708 709 710 711 712 713 714 715 716 717 718 719 720	CB CG CD1 CD2 CE1 CE2 CZ OH CA C C CB CG OD1	TYR TYR TYR TYR TYR TYR TYR TYR TYR ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	A 11 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	103 103 103 103 103 103 103 104 104 104 104	23.190 21.796 20.846 19.577 21.203 18.696 20.325 19.070 18.183 24.725 25.752 25.735 26.079 27.089 28.233 28.069	27.732 30.599 29.663 29.445 29.010 28.587 28.153 27.947 27.099 29.345 28.444 28.408 29.388 28.931 28.037 27.137	41.165 41.706 42.385 41.868 43.553 42.483 44.189 43.647 44.264 41.391 41.873 43.394 44.062 41.350 41.731 42.605	1.00 31.11 1.00 30.75 1.00 31.98 1.00 36.08 1.00 36.91 1.00 37.42 1.00 37.63 1.00 38.74 1.00 40.90 1.00 30.34 1.00 30.04 1.00 29.73 1.00 28.53 1.00 30.02 1.00 28.92	000000000000000000000000000000000000000
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	705 706 707 708 709 710 711 712 713 714 715 716 717 718 719 720 721	CB CG CD1 CD2 CE1 CE2 CZ OH N CA C O CB CG OD1 OD2	TYR TYR TYR TYR TYR TYR TYR TYR TYR TYR	A 11 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	103 103 103 103 103 103 104 104 104 104 104	23.190 21.796 20.846 19.577 21.203 18.696 20.325 19.070 18.183 24.725 25.752 25.735 26.079 27.089 28.233 28.069 29.339	27.732 30.599 29.663 29.445 29.010 28.587 28.153 27.947 27.099 29.345 28.444 28.408 29.388 28.931 28.037 27.137 28.183	41.165 41.706 42.385 41.868 43.553 42.483 44.189 43.647 44.264 41.391 41.873 43.394 44.062 41.350 41.731 42.605 41.168	1.00 31.11 1.00 30.75 1.00 31.98 1.00 36.08 1.00 36.91 1.00 37.42 1.00 37.63 1.00 38.74 1.00 40.90 1.00 30.34 1.00 30.04 1.00 29.73 1.00 28.53 1.00 30.07 1.00 30.02 1.00 28.92 1.00 29.24	000000000000000000000000000000000000000
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	705 706 707 708 709 710 711 712 713 714 715 716 717 718 719 720	CB CG CD1 CD2 CE1 CE2 CZ OH CA C C CB CG OD1	TYR TYR TYR TYR TYR TYR TYR TYR TYR ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	A 11 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	103 103 103 103 103 103 104 104 104 104 104	23.190 21.796 20.846 19.577 21.203 18.696 20.325 19.070 18.183 24.725 25.752 25.735 26.079 27.089 28.233 28.069	27.732 30.599 29.663 29.445 29.010 28.587 28.153 27.947 27.099 29.345 28.444 28.408 29.388 28.931 28.037 27.137	41.165 41.706 42.385 41.868 43.553 42.483 44.189 43.647 44.264 41.391 41.873 43.394 44.062 41.350 41.731 42.605	1.00 31.11 1.00 30.75 1.00 31.98 1.00 36.08 1.00 36.91 1.00 37.42 1.00 37.63 1.00 38.74 1.00 40.90 1.00 30.34 1.00 30.04 1.00 29.73 1.00 28.53 1.00 30.02 1.00 28.92	000000000000000000000000000000000000000

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ATOM	723 CA				27.095		1.00 2		
MOTA	724 C		A 105	26.461	27.343		1.00 2 1.00 2		
MOTA	725 0		A 105	26.412	27.872		1.00 2		
MOTA	726 CE		A 105	24.601	25.699	45.672 45.410	1.00 3		
MOTA	727 CC			23.097	25.621 24.210	45.410	1.00 3		
MOTA	728 CI		A· 105	22.546	23.320	46.072	1.00 3		
ATOM			A 105	22.945 21.683	24.001	44.402	1.00 3		
ATOM		E2 GLU		27.607	27.000	45.565	1.00 2		
ATOM	731 N		A 106	28.897		46.243	1.00 2		
ATOM	732 C		A 106 A 106	29.245	28.608	46.493	1.00 2		
ATOM	733 C		A 106 A 106	30.051	28.903	47.363	1.00 2		
ATOM	734 O 735 C		A 106 .	30.036	26.530	45.433	1.00 2		
MOTA			A 106	29.864	25.036	45.094	1.00 3		•
MOTA	736 C		A 107	28.646	29.516	45.724	1.00 2		
MOTA	738 C		A 107	28.925	30.933	45.876	1.00 2		
ATOM	739 C		A 107	27.933	31.605	46.820	1.00		
MOTA MOTA	740 O		A 107	28.062	32.785	47.100	1.00		
ATOM			A 107	28.924	31.636	44.504	1.00	29.35	
MOTA			A 107	30.222	31.411	43.697	1.00	28.97	
MOTA			A 107	30.142	31.864	42.230	1.00		
ATOM			A 107	31.459	31.534	41.498	1.00		
ATOM			A 107	31.578	32.052	40.083	1.00		
MOTA	746 N		A 108	26.950	30.869	47.320	1.00		
MOTA			A 108	25.939	31.482	48.186	1.00		
MOTA	748 C		A 108	26.468	32.050	49.514		33.50	
MOTA			A 108	25.987	33.082	49.988		33.27	
MOTA		CB MET	A 108	24.787	30.509	48.417		33.11	
MOTA			A 108	23.976	30.300	47.127		34.43	
MOTA		SD MET	A 108	22.458	29.330	47.263		37.47	
ATOM			A 108	21.487	30.326			37.24	
MOTA	754 ì	N ALA	A 109	27.484	31.427	50.090		34.73	
ATOM	· 755 (A 109	28.039	31.922	51.359	1.00		
MOTA	756		A 109	28.555	33.361	51.266		37.12 37.35	
MOTA			A 109	28.455	34.127	52.213			
MOTA			A 109	29.147	30.991	51.860		35.96 38.70	•
MOTA			A 110	29.076	33.745	50.112		39.61	
MOTA			A 110	29.631		49.949		39.61	
MOTA			A 110	28:605				39.50	
MOTA			A 110	28.950				39.94	
MOTA			A 110	30.730 31.916		• •		41.54	
MOTA			I A 110	32.341				41.36	
MOTA		OD1 ASN		32.451				43.06	
MOTA			E A 111	27.349				40.12	
ATOM. ATOM			E A 111	26.278				40.43	
MOTA			E A 111	25.064				41.38	•
ATOM	770		E A 111	24.068				40.89	
ATOM	771		E A 111	25.954				40.30	•
MOTA	772		E A 111	26.973				38.60	
ATOM	773		E A 111	28.199			1.00	37.50	
ATOM	774		E A 111	26.705				38.02	
ATOM	775		E A 111	29.140			1.00	36.74	
MOTA	776		E A 111	27.649				36.60	
ATOM	777		E A 111	28.863		5 45.433		35.45	
MOTA	778		N A 112	25.175	36.457			42.72	
ATOM	779		N A 112	24.154				43.86	
ATOM	780		N A 112	22790				44.00	•
ATOM	781	O GL	N A 112	21.774				44.39.	
MOTA	782		N A 112	24.535				44.29	
MOTA	783		N A 112	25.923	35.98	5 54.166	1.00	46.45	

ATOM	784 CD	GLN A 112	26.050	34.477	54.296	1.00 49.14	С
MOTA	785 OE1	GLN A 112	25.523	33.733	53.466	1.00 50.83	0
ATOM	786 NE2			34.022	55.332	1.00 50.52	N
ATOM	787 N	ASN A 113	22.765	37.759	51.299	1.00 43.96	N
ATOM	788 CA	ASN A 113	21.504	38.416	50.971	1.00 44.15	C
ATOM	789 C	ASN A 113	20.827	37.921	49.679	1.00 44.12	Ċ
ATOM	790 O	ASN A 113	19.768	38.431	49.309	1.00 44.11	ō
			21.696	39.941	50.918	1.00 44.21	c
ATOM	791 CB	ASN A 113			52.283		c
MOTA	792 CG	ASN A 113	22.084	40.541		1.00 44.80	
MOTA		ASN A 113	21.759	39.991	53.349	1.00 43.65	0
ATOM		2 ASN A 113	22.778	41.675	52.246	1.00 44.92	N
ATOM	795 N	PHE A 114	21.415	36.939	48.995	1.00 43.98	N
MOTA	796 CA	PHE A 114	20.793	36.411	47.787	1.00 43.71	C
ATOM	797 C	PHE A 114	19.778	35.345	48.150	1.00 43.76	C
MOTA	798 O	PHE A 114		34.362	48.815	1.00 43.32	0
ATOM	799 CB	PHE A 114	21.813	35.808	46.833	1.00 43.82	С
ATOM	800 CG	PHE A 114	21.184	35.128	45.650	1.00 43.80	С
MOTA		1 PHE A 114	20.567	35.881	44.661	1.00 43.54	С
ATOM	802 CD2	2 PHE A 114	21.170	33.745	45.541	1.00 43.65	С
MOTA	803 CE	l PHE A 114	19.963	35.276	43.587	1.00 43.55	С
ATOM	804 CE	2 PHE A 114	20.566	33.129	44.451	1.00 43.21	С
ATOM	805 CZ	PHE A 114	19.961	33.897	43.476	1.00.42.89	С
ATOM	806 N	LYS A 115	18.543	35.543	47.705	1.00 43.96	N
ATOM	807 CA	LYS A 115	17.459	34.613	47.999	1.00 44.38	C
ATOM	808 C	LYS A 115	16.933	34.026	46.693	1.00 44.04	C
ATOM	809 O	LYS A. 115	16.213	34.687	45.945	1.00 43.97	0
ATOM	810 CB	LYS A 115	16.342	35.329	48.761	1.00 44.79	С
ATOM	811 CG	•	16.763	35.866	50.129	1.00 46.74	С
ATOM	812 CD		17.021	34.744	51.130	1.00 48.83	С
MOTA	813 CE		17.461	35.288	52.484	1.00 50.18	С
ATOM	814 NZ		17.498	34.224	53.539	1.00 51.05	N
ATOM	815 N	PRO A 116	17.270	32.771	46.433	1.00 43.65	· N
ATOM	816 CA		16.918	32.133	45.160	1.00 43.43	C
ATOM	817 C	PRO A 116	15.415	32.034	44.969	1.00 42.76	С
ATOM	818 O	PRO A 116	14.711	31.724	45.915	1.00 42.78	0
ATOM	819 CB		17.525	30.732	45.273	1.00 43.57	· C
ATOM	820 CG		18.385	30.743	46.496	1.00 43.88	·C
MOTA	821 CD		17.948	31.855	47.359	1.00 43.68	C
ATOM	822 N	ARG A 117	14.940	32.306	43.761	1.00 42.20	N
ATOM	823 CA		13.518	32.214	43.451	1.00 41.56	C
. ATOM	824 C	ARG A 117	13.140	30.780	43.104	1.00 41.00	Č
ATOM	825 · O	ARG A 117	11.957	30.461		1.00 41.15	Ö
ATOM	826 CE		13.164	33.132	42.311	1.00 41.47	c
ATOM	827 N		14.139	29.925	42.904		N
ATOM	828 C		13.882	28.517	42.654		c
ATOM	829 C	SER A 118	14.700	27.655	43.621		c
			15.756	28.078	44.087		o
ATOM							C
ATOM			14.184	28.158	41.196 40.942		o
ATOM	832 O		15.560	28.228			N
ATOM	833 N		14.180	26.471	43.943		
ATOM	834 C			25.537			C
ATOM	835 C		15.115	24.215	44.160		C
ATOM	836 0		14.314	23.751	43.359		0
ATOM	837 C		13.958	25.220	46.068		C
ATOM	838 C		13.466				C
ATOM		D1 ASN A 119	14.255				0
MÓTA		D2 ASN A 119	12.145		46.906		N
MOTA	841 N		16.243		44.492		N
MOTA		A ARG A 120	16.627				C
ATOM	843 C		16.209				C
MOTA	844 O	ARG A 120	16.359	21.272	46.069	1.00 37.28	. 0

ATOM	845	СВ	ARG :	A	120	18.144		22.264	43.730	1.00	37.07		С
ATOM	846	CG	ARG .			18.632		21.020	42.993	1.00	36.32		С
ATOM	847	CD	ARG .			20.152		20.886	42.938		35.46		С
ATOM	848	NE	ARG .			20.777		21.277	44.198		34.29		N
MOTA	849	CZ	ARG .			21.049		20.445	45.202		36.66		C
ATOM	850		ARG .			20.753		19.147	45.122		35.60		N
ATOM	851		ARG			21.614		20.915	46.305		37.13		N
ATOM	852	N CA	GLU GLU			15.665 15.326		20.141 18.944	44.250		36.76		N
ATOM ATOM	853 854	CA	GLU			15.810		17.746	44.993 44.187		36.29		C
ATOM	855	0	GLU			15.709		17.726	42.953		35.35 35.38		0
ATOM	856	СВ	GLU			13.820		18.863	45.262		36.78		c
ATOM	857	CG	GLU			13.398		17.585	45.971		39.29		C.
ATOM	858	CD	GLU			12.126		17.732	46.795		42.09		č
ATOM	859		GLU			12.200		18.310	47.904		45.56		. 0
ATOM	860	OE2				11.059		17.254	46.350		43.04		ō
ATOM	861	N	GLÜ			16.366		16.764		1.00			N
ATOM	862	CA	GLU			16.840		15.547	44.266	1.00	33.04		С
MOTA	863	С	GLU	Α	122	15.748	3	14.518	44.415	1.00	32.55		С
ATOM	864	0	GLU			15.253		14.306	45.511	1.00	32.52	_	0
MOTA	865	CB	GLU			18.103		15.052	44.961	1.00	32.71	•	С
ATOM	866	CG	GLU			19.265		16.018	44.885	1.00	31.86		С
ATOM	867	CD	GLU			19.705		16.296	43.454	1.00	31.04		C
ATOM	868		GLU			20.065		15.331	42.757		29.68		0
MOTA	869		GLU			19.694		17.479	43.025	1.00			0
ATOM	870	N	MET			15.349		13.885	43.321	1.00	31.83		N
ATOM	871 872	CA C	MET			14.329		12.858	43.415	1.00			C
ATOM ATOM	873	0	MET MET			14.532 15.380		11.820 11.982	42.343 41.457	1.00	30.68 30.07		C
ATOM	874	СВ	MET			12.93		13.466	43.309		31.52		O C.
ATOM	875	CG	MET			12.66		14.205	42.032		32.93		c.
ATOM	876	SD	MET			11.11		15.145	42.034	1.00			s
MOTA	877	CE			123	11.55		16.565	42.966		35.33		c
ATOM	878	N			124	13.76		10.738	42.464		29.85		N
MOTA	879	CA			124	13.75		9.671	41.483		29.22		С
MOTA	880	С	LYS	A	124	12.89	1	10.140	40.307	1.00	28.45		С
MOTA	881	0	LYS	A	124	12.06	6	11.039	40.466	1.00	27.39		0
MOTA	882	CB	LYS	Α	124	13.18	3	8.389	42.100	1.00	29.57		С
MOTA	883	CG			124	13.95		7.857	43.321		29.88		С
ATOM	884	CD			124	15.39		7.501	42.950		30.48		С
ATOM	885	CE			124	16.23		7.129	44.167	1.00			С
ATOM	886	NZ			124	17.69		7.276	43.872		30.47		N
ATOM	887	N			125	13.07		9.536	39.133		27.71		N
MOTA	888	CA			125	12.36		10.000	37.949		27.22		C
MOTA MOTA	889 890	C O			125 125	10.86 10.13		9.891 10.825	38.114 37.801		27.29 26.75		C
ATOM	891	CB			125	12.79		9.270	36.681		26.75		0 C
ATOM	892	CG			125	12.49		10.051	35.433		27.63		C
ATOM	893		PHE			13.33		11.083	35.032		27.70		č
MOTA	894		PHE			11.35		9.802	34.702		28.29		Č
ATOM	895		PHE			13.05		11.828	33.905		27.96	•	Ċ
ATOM	896		PHE			11.06		10.540	33.563		29.16		c
MOTA	897	CZ			125	11.92		11.568	33.167		28.71		С
MOTA	898	N	HIS	A	126	10.42		8.743	38.620	1.00	27.46		N
ATOM	899	CA	HIS	A	126	9.01	3	8.499	38.832	1.00	27.77		С
ATOM	900	С			126	8.43		9.522	39.794	1.00	27.71		С
MOTA	901	0			126	7.24		9.821	39.731		27.27		0
ATOM	902	CB			126	8.77		7.056	39.329		27.96		C
ATOM	903	CG			126	8.89		6.880	40.812		28.47		C
ATOM	904		HIS			7.83		7.026	41.672		29.29		N
MOTA	905	CD2	HIS	A	126	9.96	1	6.552	41.585	1.00	29.43		С

ATOM	906	CE1	HIS A	126	8.236	6.812	42.912	1.00 30.2	26	С
ATOM	907		HIS A		9.525	6.524	42.887	1.00 29.6		N
ATOM	908		GLU A		9.262	10.059	40.679	1.00 28.0		N
MOTA	909		GLU A		8.803	11.078	41.615	1.00 28.0		C
ATOM	910		GLU A		8.585	12.400	40.865	1.00 28.9		Ċ
	911		GLU A		7.626	13.129	41.123	1.00 29.3		Ō
MOTA	912		GLU A		9.795	11.233	42.775	1.00 28.		Č
ATOM			GLU A		9.931	9.968	43.626	1.00 29.		Č
ATOM	913					10.121	44.810	1.00 30.		č
ATOM	914	CD	GLU A		10.873	10.121	44.603	1.00 30.		Ö
ATOM	915		GLU A		12.069	9.943		1.00 23.		. 0.
ATOM	916		GLU A		10.410		45.962			. O.
MOTA	917	N	PHE A		9.471	12.696	39.927	1.00 29.		C
ATOM	918	CA	PHE A		9.354	13.914	39.119	1.00 29.		C
ATOM '	919	С	PHE A		8.047	13.859	38.333	1.00 30.		
MOTA	920	0	PHE A		7.274	14.817	38.294	1.00 29.		0
ATOM	921	CB	PHE A		10.551	14.017	38.167	1.00 29.		C
MOTA	922	CG	PHE A		10.337	14.950	36.991	1.00 28.		C
ATOM	923	CD1	PHE A	128	10.106	16.301	37.188	1.00 26.		C
MOTA	924	CD2	PHE A	128	10.397	14.475	35.696	1.00 26.		C
MOTA.	925	CE1	PHE A	128	9.920	17.149	36.120	1.00 27.		C
MOTA	926	CE2	PHE A	128	10.217	15.341	34.610	1.00 28.		С
ATOM	927	CZ	PHE A	128	9.976	16.668	34.823	1.00 26.		С
ATOM	928	N	VAL A	129	7.797	12.705	37.736	1.00 31.		N
MOTA	929	CA	VAL A	129	6.603	12.499	36.930	1.00 32.		С
ATOM	930	С	VAL A	12.9	5.338	12.658	37.775	1.00 32.	96	С
MOTA	931	0	VAL A	129	4.398	13.362	37.388	1.00 32.	79	0
MOTA	932	CB	VAL A	129	6.606	11.094	36.313	1.00 32.	48	C.C
MOTA	933	CG1	VAL A	129	5.313	10.840	35.551	1.00 32.	96	С
ATOM	934		VAL A		7.828	10.901	35.417	1.00 31.	98	С
ATOM	935	N	GLU A		5.329	11.993	38.925	1.00 33.	61	N
ATOM	936	CA	GLU A		4.205	12.067	39.853	1.00 34.	29	С
ATOM	937	C	GLU A		3.963	13.515	40.246	1.00 34.	51	. C
ATOM	938	ŏ	GLU A		2.832	13.986	40.220	1.00 33.		0
ATOM	939	СВ	GLU A		4.481	11.206	41.087	1.00 34	. 35	С
ATOM	940	CG	GLU A		4.372	9.711	40.815	1.00 34		С
ATOM	941	CD	GLU A		5.204	8.858	41.761	1.00 35		. С
ATOM	942		GLU A		5.595	9.345	42.845	1.00 36		0
ATOM	943		GLU A		5.477	7.692	41.407	1.00 36		0
MOTA	944	N	LYS A		5.033	14.223	40.587	1.00 35		N
MOTA	945	CA	LYS A		4.912	15.632	40.920	1.00 36		C
MOTA	946	C	LYS A		4.286	16.408	39.758	1.00 36		С
ATOM	947	o	LYS A		3.420	17.253	39.972	1.00 36		Ō
ATOM	948	СВ	LYS A		6.269	16.240	41.261	1.00 36		C
ATOM	949	CG	LYS A		6.467	16.623	42.712	1.00 37		Č
ATOM	950	· CD	LYS A		7.125	18.001	42.822	1.00 38		Ċ
			LYS A		7.123	18.324	44.252	1.00 40		c
ATOM	951	CE	LYS A			19.747	44.404	1.00 40		Ŋ
ATOM	952	NZ			8.073	16.142	38.532	1.00 37		N
ATOM	953	N	LEU A		4.725		37.383	1.00 37		C
ATOM	954	CA	LEU A		4.156					č
ATOM	955	С	LEU A		2.669		37.280	1.00 38		o
ATOM	956		LEU A		1.875		36.976	1.00 38		C
MOTA	957		LEU P		4.819		36.081			
MOTA	958		LEU F		6.224			1.00 39		C
MOTA	959		LEU F		6.671					C
ATOM	960		2 LEU F		6.281					
MOTA	961		GLN A		2.311					. И
MOTA	962		GLN A		0.920					C
MOTA	963		GLN A		0.057					C
MOTA	964		GLN A		-1.035					0
ATOM	965		GLN A		0.835					C
MOTA	966	N	ASP A	A: 134	0.542	15.682	39.777	1.00 41	.89	N

ATOM	967	CA	ASP .	A	134	-0.232	16.313	40.854	1.00 42.72	С
ATOM	968	С	ASP .	A	134	-0.506	17.792	40.576	1.00 42.60	С
ATOM	969	0	ASP			-1.570	18.316	40.900	1.00 42.25	0
MOTA	970	CB	ASP			0.491	16.169	42.200	1.00 43.21	C
ATOM	971	CG	ASP			-0.429	16.419	43.396	1.00 45.71	С
ATOM	972		ASP			-1.566	16.916	43.213	1.00 48.39	0
ATOM ATOM	973 974		ASP ILE			-0.104 0.467	16.131 18.467	44.571 39.981	1.00 49.60 1.00 42.77	. О
ATOM	975	N CA	ILE			0.306	19.872	39.660	1.00 42.77	C
MOTA	976	C	ILE			-0.793	20.050	38.626	1.00 43.15	č
ATOM	977	ŏ	ILE			-1.690	20.871	38.800	1.00 43.03	ŏ
ATOM	978	СВ	ILE			1.623	20.443	39.155	1.00 42.94	. C
MOTA	979	CG1	ILE			2.586	20.607	40.330	1.00 43.10	C
MOTA	980	CG2	ILE	A	135	1.396	21.778	38.473	1.00 42.80	С
MOTA	981	CD1	ILE			4.040	20.621	39.934	1.00 43.49	C
MOTA	982	N	GLN			-0.716	19.272	37.554	1.00 43.64	N
MOTA	983	CA	GLN			1.712	19.321	36.496	1.00 44.17	C
MOTA	984	C	GLN			-3.103	19.129	37.081	1.00 44.65	C
MOTA	985	0	GLN			-3.976	19.984	36.936	1.00 44.71	0
ATOM ATOM	986 987	CB N	GLN GLN			-1.431 -3.289	18.240 18.014	35.466 37.776	1.00 44.19 1.00 45.23	C N
MOTA	988	CA	GLN			-4.596	17.654	38.314	1.00 45.25	C
ATOM	989	C	GLN			-5.146	18.696	39.277	1.00 45.88	č
ATOM	990	ō	GLN			-6.337	19.005	39.238	1.00 46.33	ō
MOTA	991	СВ	GLN			-4.535	16.277	38.991	1.00 45.74	С
MOTA	992	N	ARG	Α	138	-4.288	19.246	40.131	1.00 45.93	N
MOTA	993	CA	ARG	A	138	-4.740	20.211	41.132	1.00 45.84	C
MOTA	994	С	ARG			-4.720	21.640	40.592	1.00 45.53	С
MOTA	995	0	ARG			-4.911	22.598	41.344	1.00 45.72	0
MOTA	996	CB	ARG			-3.880	20.108	42.398	1.00 45.92	C
MOTA	997	CG	ARG			-2.551	20.866	42.340	1.00 46.84	C
ATOM ATOM	998 999	CD NE	ARG ARG			-1.589 -0.509	20.458 21.418	43.437 43.652	1.00 47.70 1.00 47.78	N
ATOM	1000	CZ			138		21.125	43.578	1.00 47.78	C
ATOM	1001		ARG			1.186	19.897	43.274	1.00 50.12	N
ATOM	1002		ARG			1.702	22.064	43.798	1.00 49.52	N
ATOM	1003	N			139	-4.492	21.783	39.290	1.00 44.99	Ŋ
MOTA	1004	CA			139	-4.419	23.094	38.669	1.00 44.52	С
ATOM	1005	С			139	-3.412	.24.041	39.310	1.00 44.06	С
MOTA	1006	0			139	-3.551	25.259	39.203	1.00 44.28	. 0
MOTA	1007	N			140	-2.382	23.495	39.953	1.00 43.28	N
ATOM	1008	CA			140	-1.388		40.629	1.00 42.49	C
ATOM ATOM	1009 1010	C O			140 140	-0.609 -0.556	25.218 24.989	39.694 38.480	1.00 41.92 1.00 41.85	C 0
MOTA	1010	N			141	-0.004	26.264	40.250	1.00 41.83	N
ATOM	1012	CA.			141	0.789	27.186	39.444	1.00 40.07	C
ATOM	1013	C			141	2.286	26.884	39.549	1.00 38.68	C
ATOM	1014	0.			141	3.096	27.503	38.867	1.00 38.67	Ō
MOTA	1015	CB	GLU	Α	141	0.513	28.644	39.839	1.00 40.36	С
MOTA	1016	CG			141	-0.799	29.224	39.309	1.00 41.91	С
MOTA	1017	CD			141	-1.001	.29.042	37.805	1.00 44.25	С
MOTA	1018		GLU			0.004	29.008	37.043		. 0
ATOM	1019		GLU			-2.181	28.940	37.380		0
MOTA	1020	N CT			142	2.648	25.944	40.413		N
MOTA MOTA	1021 1022	CA C			142	4.040 4.629	25.573	40.596		C C
ATOM	1022	0			142	3.923	25.120 24.594	39.265 38.408	1.00 34.41 1.00 34.25	0
MOTA	1023	СВ			142	4.150	24.394	41.627	1.00 34.25	C
ATOM	1025	CG			142	5.571	24.173	42.095		C
ATOM	1026	CD			142	5.710	22.944	42.978	1.00 36.48	Č
MOTA	1027		. GLU			4.733	22.174	43.142		0

ATOM	1028 OE2 GLU A 142	6.821 22.739 43.511 1.00 36.76	
ATOM	1029 N ARG A 143	5.926 25.323 39.096 1.00 32.91	
MOTA	1030 CA ARG A 143	6.596 24.893 37.884 1.00 31.95	
ATOM	1031 C ARG A 143	7.803 24.058 38.214 1.00 30.62	
		8.514 24.354 39.166 1.00 30.75	
MOTA	=	7.072 26.097 37.082 1.00 32.19	
MOTA		5.968 26.912 36.447 1.00 32.57	
MOTA	1034 CG ARG A 143		
MOTA	1035 CD ARG A 143		
ATOM	1036 NE ARG A 143		
MOTA	1037 CZ ARG A 143	5.158 28.617 33.790 1.00 31.80	
MOTA	1038 NH1 ARG A 143	5.757 27.637 33.105 1.00 31.28	
MOTA	1039 NH2 ARG A 143	4.214 29.345 33.221 1.00 32.77	
ATOM	1040 N LEU A 144	8.054 23.028 37.417 1.00 28.97	
ATOM	1041 CA LEU A 144	9.235 22.219 37.617 1.00 28.09	
ATOM	1042 C LEU A 144	10.150 22.257 36.398 1.00 27.14	
MOTA	1043 O LEU A 144	9.690 22.418 35.272 1.00 26.74	
ATOM	1044 CB LEU A 144	8.834 20.783 37.887 1.00 28.28	
MOTA	1045 CG LEU A 144	7.839 20.606 39.038 1.00 28.89	
	1046 CD1 LEU A 144	7.515 19.123 39.216 1.00 29.62	
ATOM		8.364 21.212 40.333 1.00 27.84	
ATOM		11.447 22.102 36.636 1.00 25.69	
MOTA		12.395 21.976 35.548 1.00 25.05	
MOTA	 	13.459 20.957 35.968 1.00 25.00	
MOTA	1050 C TYR A 145	14.239 21.193 36.881 1.00 25.01	
MOTA	1051 O TYR A 145		
MOTA	1052 CB TYR A 145		
MOTA	1053 CG TYR A 145		
ATOM	1054 CD1 TYR A 145	13.739 22.385 32.931 1.00 21.70	
MOTA	1055 CD2 TYR A 145	13.667 24.746 33.175 1.00 22.16	
MOTA	1056 CE1 TYR A 145	14.154 22.526 31.620 1.00 20.98	
MOTA	1057 CE2 TYR A 145	14.097 24.904 31.846 1.00 21.30	
ATOM	1058 CZ TYR A 145	14.332 23.799 31.071 1.00 20.66	
MOTA	1059 OH TYR A 145	14.737 23.933 29.740 1.00 18.43	
MOTA	1060 N LEU A 146	13.446 19.808 35.318 1.00 24.9	
MOTA	1061 CA LEU A 146	14.453 18.787 35.547 1.00 25.43	
MOTA	1062 C LEU A 146	15.678 19.100 34.694 1.00 24.93	1
MOTA	1063 O LEU A 146	15.555 19.313 33.493 1.00 24.1	0
MOTA	1064 CB LEU A 146	13.907 17.419 35.162 1.00 25.5	9
MOTA	1065 CG LEU A 146	14.875 16.238 35.334 1.00 27.5	2
		14.111 14.966 35.672 1.00 26.9	
MOTA		15.742 16.023 34.084 1.00 29.4	
ATOM		16.845 19.097 35.330 1.00 24.9	
ATOM		18.115 19.394 34.685 1.00 25.2	
ATOM		19.146 18.490 35.317 1.00 25.2	
MOTA	1070 C GLN A 147		
MOTA	1071 O GLN A 147		
MOTA	1072 CB GLN A 147		
MOTA		# · · · · · · · · · · · · · · · · · · ·	
MOTA			
ATOM		16.891 24.149 34.141 1.00 27.9	
MOTA	1076 NE2 GLN A 147	18.860 23.575 35.064 1.00 23.5	
MOTA	1077 N GLNA 148	19.487 17.428 34.611 1.00 25.4	
ATOM	1078 CA GLN A 148	20.319 16.365 35.146 1.00 25.4	
ATOM		21.254 15.816 34.105 1.00 25.5	
ATOM		20.862 15.485 32.992 1.00 25.0	
ATOM		19.436 15.231 35.640 1.00 25.3	
ATOM		20.201 14.021 36.167 1.00 26.1	
ATOM		21.129 14.383 37.314 1.00 26.5	
ATOM		20.718 15.093 38.240 1.00 23.9	94
ATOM		22.383 13.916 37.248 1.00 25.2	
		22.510 15.769 34.482 1.00 25.8	
ATOM		23.552 15.219 33.667 1.00 27.0	
ATOM		23.298 13.720 33.527 1.00 27.3	
ATOM	1 1000 C 1HK W 143	23.250 201.25 20.00	

ATOM	1089	0	THR A	149	23.012	13.044	34.508	1.00 26.86	0
ATOM	1090	CB	THR A	149	24.903	15.540	34.375	1.00 27.42	С
MOTA	1091	OG1	THR A	149	25.300	16.882	34.020	1.00 29.80	0
MOTA	1092	CG2	THR A	149	26.034	14.702	33.873	1.00 28.98	С
MOTA	1093	N	LEU A		23.338	13.224	32.298	1.00 27.70	N
ATOM	1094	CA	LEU A		23.195	11.812	32.027	1.00 28.46	С
MOTA	1095	С	LEU A		24.429	11.076	32.573	1.00 28.97	С
ATOM	1096	0	LEU A		25.548	11.468	32.268	1.00 29.00	0
ATOM	1097	CB	LEU A		23.084	11.580	30.524	1.00 28.34	C
ATOM	1098	CG	LEU A		21.780	11.981	29.837	1.00 29.63	C
ATOM	1099	CD1	LEU A		21.944	11.862	28.328	1.00 30.03	C
ATOM	1100		ĻEU A		20.619	11.140	30.310	1.00 31.15	C
MOTA	1101	N	ASN A		24.230	10.030	33.378	1.00 29.35	N
MOTA	1102	CA	ASN A		25.348	9.258	33.949	1.00 29.51	C
ATOM	1103	C	ASN A		25.137	7.732	33.934	1.00 29.92	C
ATOM ATOM	1104 1105	O CB	ASN A		24.162 25.590	7.241 9.710	33.348 35.385	1.00 29.73 1.00 29.78	0 C
. ATOM	1105	CG	ASN A		24.362	9.553	36.241	1.00 29.78	C
ATOM	1107		ASN A		23.735	8.497	36.241	1.00 29.19	0
ATOM	1108	ND2			23.733	10:611	36.200	1.00 30.03	N
ATOM	1109	N	ASP A		26.020	6.999	34.627	1.00 29.31	N
ATOM	1110	. CA	ASP A		26.034	5.514	34.649	1.00 30.27	C
ATOM	1111	C	ASP A		24.830	4.797	35.212	1.00 30.55	Ċ
ATOM	1112	<u>o</u> .	ASP A		24.779	3.562	35.137	1.00 30.29	Ö
ATOM	1113	СВ	ASP A		27.178	4.965	35.519	1.00 31.48	Ċ
ATOM	1114	CG	ASP A		28.384	5.812	35.493	1.00 34.64	Ċ
MOTA	1115	OD1	ASP A		28.588	6.523	34.482	1.00 41.71	. 0
MOTA	1116		ASP A		29.177	5.857	36.437	1.00 37.31	0
ATOM	1117	N	THR A		23.894	5.501	35.833	1.00 30.21	N
ATOM	1118	CA	THR A	153	22.767	4.785	36.432	1.00 30.13	С
MOTA	1119	С	THR A	153	21.612	4.626	35.463	1.00 29.54	С
MOTA	1120	0	THR A	. 153	20.639	3.970	35.778	1.00 29.38	0
MOTA	1121	CB	THR A	. 153	22.277	5.481	37.704	1.00 30.37	С
MOTA	1122	OG1			21.735	6.770	37.373	1.00 31.06	0
MOTA	1123	CG2			23.452	5.763	38.658	1.00 30.56	С
MOTA	1124	N	VAL A		21.703	5.213	34.280	1.00 29.07	N
MOTA	1125	CA	VAL A		20.596	5.082	33.346	1.00 28.90	С
MOTA	1126	С	VAL A		20.488	3.613	32.968	1.00 28.83	С
ATOM	1127	0	VAL A		21.486	2.898	33.002	1.00 28.78	0
ATOM	1128	CB	VAL A		20.762	5.952	32.088	1.00 28.61	C
MOTA	1129		VAL A		20.808	7.410	32.462	1.00 29.14	C
MOTA	1130		VAL A		21.999	5.547	31.305	1.00 28.52	C
MOTA MOTA	1131	N	GLY A		19.283	3.170	32.615	1.00 28.74	N
ATOM	1132 1133	CA C	GLY A		19.043 19.484	1.780	32.263	1.00 28.33	C
ATOM	1134	0	GLY A		19.862	1.387 2.235	30.860 30.031	1.00 28.70 1.00 28.27	.C
ATOM	1135	N	ARG A		19.384	0.088	30.591	1.00 28.27	O N
ATOM	1136	CA	ARG A		19.857	-0.519	29.349	1.00 28.47	И С
ATOM	1137	C	ARG A		19.291	0.096	28.084	1.00 28.18	c
ATOM	1138	ŏ	ARG A		20.029	0.346	27.143	1.00 28.69	o
ATOM	1139	СВ	ARG A		19.582	-2.019	29.362	1.00 28.58	č
ATOM	1140	N	LYS P		17.986	0.304	28.042	1.00 27.53	N
ATOM	1141	CA	LYS A		17.390	0.888	26.860	1.00 27.32	c
MOTA	1142	C	LYS A		17.947	2.306	26.625	1.00 27.10	č
ATOM .		ō	LYS A		18.213	2.672	25.490	1.00 26.76	ő
ATOM	1144	СВ	LYS A		15.858	0.902	26.960	1.00 27.68	č
ATOM	1145	CG	LYS F		15.171	-0.451	26.656	1.00 26.26	Ċ
MOTA	1146	N	ILE F		18.138	3.086	27.688	1.00 26.68	N
ATOM	1147	CA	ILE A		18.665	4.450	27.543	1.00 26.67	С
MOTA	1148	С	ILE A	158	20.107	4.368	27.100	1.00 26.53	С
MOTA	1149	0	ILE A	158	20.558	5.170	26.285	1.00 25.74	0
					,				

ATOM	1150	CB	ILE A 158	18.570	5.245	28.837	1.00 26.51		C
ATOM	1151		ILE A 158	17.114	5.399	29.269	1.00 27.11		С
MOTA	1152	CG2	ILE A 158	19.208	6.618	28.667	1.00 27.55		С
MOTA	1153	CD1	ILE A 158	16.232	6.028	28.260	1.00 28.98		С
MOTA	1154	N	VAL A 159	20.817	3.378	27.629	1.00 26.46		N
MOTA	1155		VAL A 159	22.187	3.125	27.226	1.00 26.70		·C
MOTA	1156		VAL A 159	22.191	2.813	25.728	1.00 26.30		C
MOTA	1157		VAL A 159	. 23.022	3.332	24.999	1.00 25.90		. 0
MOTA	1158		VAL A 159	22.819	1.963	28.018	1.00 27.18		C
MOTA	1159		VAL A 159	24.045	1.436	27.311	1.00 28.12		C
MOTA	1160		VAL A 159	23.180	2.410	29.427	1.00 27.44		C
ATOM	1161		MET A 160	21.255	1.984	25.269	1.00 26.08		N C
ATOM	1162		MET A 160	21.175	1.652	23.840	1.00 26.30		C
ATOM	1163	C	MET A 160.		2.929	23.005	1.00 24.71		0
ATOM .	1164	0	MET A 160	21.559	3.164	22.000	1.00 23.40 1.00 26.71		c
ATOM	1165	CB	MET A 160	20.081	0.617	23.565 24.070	1.00 20.71		c
ATOM	1166	CG	MET A 160	20.401	-0.790 -1.628	23.154	1.00 35.73		s
ATOM	1167	SD	MET A 160	21.721 20.883	-1.823	21.524	1.00 35.73	•	C
ATOM	1168	CE	MET A 160 ASP A 161	19.948	3.739	23.439	1.00 23.86		N
ATOM	1169 1170	N CA	ASP A 161	19.636	5.000	22.756	1.00 23.67		C
ATOM		CA	ASP A 161	20.840	5.943	22.750	1.00 23.67		č
ATOM	1171 1172	0	ASP A 161	21.148	6.478	21.593	1.00 23.02		ŏ
ATOM ATOM	1172	CB	ASP A 161	18.472		23.455	1.00 23.42		Ċ
ATOM	1174	CG	ASP A 161	17.178	4.898	23.369	1.00 24.19		Ċ
ATOM	1175		ASP A 161	17.095	3.941	22.552	1.00 19.47		Ö
ATOM	1175		ASP A 161	16.197	5.164	24.087	1.00 24.90		Ö
ATOM	1177	N	PHE A 162	21.513	6.132	23.791	1.00 21.70		N
	1178	CA	PHE A 162	22.667	7.003	23.903	1.00 21.16		C
ATOM ATOM	1179	CA	PHE A 162	23.777	6.557	22.964	1.00 20.02		Ċ
ATOM	1180	0	PHE A 162	23	7.362	22.310	1.00 20.22		ō
ATOM	1181	СВ	PHE A 162		7.010	25.364	1.00 21.38		Č
ATOM	1182	CG	PHE A 162		7.936	25.650	1.00 22.82		Ċ
ATOM	1183		PHE A 162		9.290	25.882	1.00 26.05		С
ATOM	1184		PHE A 162		7.450	25.738		•	c·
ATOM	1185		PHE A 162		10.136	26.181	1.00 25.32		С
ATOM	1186		PHE A 1:62		8.301	26.026	1.00 24.73		С
ATOM	1187	CZ	PHE A 162		9.622	26.250	1.00 24.82		С
ATOM	1188	N	LEU À 163		5.271	22.894	1.00 19.74		N
ATOM	1189	CA	LEU A 163		4.767	21.998	1.00 19.88	•	C
MOTA	1190	С	LEU A 163		4.965	20.533	1.00 18.90		С
ATOM	1191	0.	LEU A 163		5.020	19.675	1.00 18.20		0
ATOM	1192	CB	LEU A 163		3.287	22.256	1.00 19.78		C
ATOM	1193	CG	LEU A 163	26.078	3.019	23.546	1.00 20.79	•	С
MOTA	1194	CD1	LEU A 163	26.069	1.534	23.811	1.00 21.16		· C
MOTA	1195	CD2	LEU A 163		3.567	23.456	1.00 21.66		С
MOTA	1196	N	GLY A 164	23.395	5.055	20.272	1.00 18.33		N
ATOM	1197	CA	GLY A 164	22.883	5.296	18.941	1.00 19.05		С
MOTA	1198	С	GLY A 164			18.519	1.00 19.33		С
MOTA	1199		GLY A 164				1.00 20.16		0
MOTA	1200	N	PHE A 165		7.651		1.00 18.45		N
MOTA	1201		PHE A 165				1.00 19.26		С
MOTA	1202		PHE A 165				1.00 19.34		C
MOTA	1203		PHE A 165				1.00 18.77		0
MOTA	1204		PHE A 165				1.00 19.09		C
MOTA	1205		PHE A 165				1.00 20.44		C
MOTA	1206		L PHE A 165						C
MOTA	1207		2 PHE A 165						C.
MOTA	1208		L PHE A 165						C
MOTA	1209		2 PHE A 165						C
MOTA	1210	CZ	PHE A 165	5 20.913	10.567	23.163	1.00 22.00		С

ATOM	1211	N	ASN A	1	166	24.508	10.157	17.040	1.00	19.48	N
ATOM	1212	CA	ASN A	\ :	166	25.428	10.290	15.897	1.00	20.08	С
ATOM	1213	С	ASN A	٠ ،	166	26.827	10.792	16.305	1.00	20.53	C
	1214		ASN A			27.193	11.975	16.076		20.34	Ö
ATOM											
MOTA	1215		ASN A			24.836	11.183	14.790		19.52	C
MOTA	1216	CG	ASN A	A : :	166	25.572	11.003	13.451		19.82	С
ATOM	1217	OD1	ASN A	Α :	166	26.652	10.376	13.412	1.00	18.39	0
ATOM	12:18	ND2	ASN A	Α :	166	24.987	11.528	12.350	1.00	15.25	N
ATOM	1219	N	TRP A			27.564	9.892	16.955	1.00	20.69	N
ATOM	1220	CA	TRP A			28.911	10.161	17.441		21.20	C
ATOM	1221	C	TRP A			29.858	10.404	16.270		21.35	Č
											Ö
MOTA	1222	0	TRP			30.806	11.171	16.371		21.36	
MOTA	1223	CB	TRP I			29.402	8.977	18.316		21.31	C
ATOM	1224	CG	TRP A	A.	167	28.550	8.849	19.539		21.63	С
MOTA	1225	CD1	TRP 2	Α	167	27.673	7.841	19.844	1.00	22.35	С
ATOM	1226	CD2	TRP 2	Α	167	28.433	9.808	20.591	1.00	20.88	С
ATOM	1227		TRP :			27.030	8.119	21.028	1.00	22.98	N
ATOM	1228	CE2	TRP .			27.486	9.315	21.511		21:22	С
ATOM	1229	CE3	TRP			29.054	11.036	20.863		20.14	. c
			TRP .			27.143	9.999	22.670		22.17	Č
ATOM	1230	CZ2									C
MOTA	1231	CZ3				28.693	11.724	21.990.		19.81	
MOTA	1232	CH2				27.742	11.206	22.889		21.02	С
MOTA	1233	N	ASN			29.610	9.743	15.153		21.50	N
MOTA	1234	CA	ASN	Α	168	30.464	9.927	13.991	1.00	21.77	С
ATOM	1235	С	ASN	Α	168	30.488	11.406	13.605	1.00	21.48	С
MOTA	1236	0	ASN			31.549	11.992	13.428	1.00	20.55	0
ATOM	1237	СВ	ASN			29.964	9.101	12.814		22.00	C
ATOM	1238	CG	ASN			30.856	9.236	11.584		23.99	Ċ
ATOM	1239		ASN			32.052	8.974	11.661			0
MOTA	1240	ND2	ASN			30.277	9.652	10.448		24.40	N
MOTA	1241	N	TRP	Α	169	29.302	11.995	13.484	1.00	21.28	N
MOTA	1242	CA	TRP	Α	169	29.183	13.372	13.071	1.00	21.23	C
ATOM	1243	С	TRP	Α	169	29.708	14.331	14.133	1.00	21.44	C
ATOM	1244	0	TRP	Α	169	30.450	15.258	13.822	1.00	20.50	0
ATOM	1245	СВ	TRP			27.736	13.741	12.740		21.29	C
ATOM	1246	CG	TRP			27.611	15.186			20.56	C
						27.840	15.766	11.173		19.81	c
ATOM	1247		TRP								Č
MOTA	1248		TRP			27.293	16.256	13.290		20.58	
MOTA	1249		TRP			27.641	17.124	11.253		20.45	N
MOTA	1250		TRP			27.313	17.453	12.540		21.52	С
MOTA	1251		TRP			26.951	16.324	14.636		22.34	С
MOTA	1252	CZ2	TRP	Α	169	27.036	18.705	13.102	1.00	24.24	С
ATOM	1253	CZ3	TRP	Α	169	26.690	17.558	15.195	1.00	24.93	С
ATOM	1254	CH2			169	26.728		14.423	1.00	25.53	С
ATOM	1255	N			170	29.318		15.381		21.81	N
ATOM	1256	CA			170	29.742	15.056			22.51	C
						31.245		16.755		23.07	c
ATOM	1257	C			170						
MOTA	1258	0			170	31.917		17.067		23.88	0
MOTA	1259	CB			170	28.837		17.662		21.97	С
MOTA	1260	CG1	ILE	Α	170	28.878	16.326	18.396		21.44	C
MOTA	1261	CG2	ILE	Α	170	29.262	13.894	18.581	1.00	21.76	C
MOTA	1262	CD1	ILE	Α	170	27.794	16.472	19.409	1.00	21.59	С
ATOM	1263	N			171	31.781		16.674		23.52	N
ATOM	1264	CA			171	33.209				24.55	Ċ
	1265	C			171	34.021		15.874		25.23	č
MOTA											
MOTA	1266	0			171	35.067		16.171		25.14	0
MOTA	1267	CB			171	33.626		16.949		24.52	C
MOTA	1268	. CC			171	33.095				24.45	С
ATOM	1269		ASN			32.625				23.01	0
MOTA	1270	ND2	2 ASN	Α	171	33.169	9.969	18.099	1.00	22.49	N
·ATOM	1271	N			172	33.560			1.00	25.46	N

MOM A	1272 CA I	YS A 172	34.255	14.963	13.592	1.00 26.46
		YS A 172	34.221		13.873	L.00 25.77
		SYS A 172	35.224		13.681	L.00 25.85
ATOM		LYS A 172	33.705	14.634		1.00 26.90
MOTA		LYS A 172	34.262	13.351		1.00 29.88
MOTA		LYS A 172	33.752	13.033		1.00 34.20
MOTA		LYS A 172	34.458	11.810		1.00 36.15
ATOM		LIS A 172	34.556	11.800		1.00 40.56
MOTA		LYS A 172	33.088	16.986		1.00 25.37
MOTA		GLN A 173	32.981	18.400		1.00 25.52
MOTA		G	34.002	18.741		1.00 25.71
MOTA		GLN A 173	34.780	19.669		1.00 26.05
MOTA		GLN A 173		18.740		1.00 25.30
MOTA		GLN A 173	31.589			1.00 25.28
MOTA	-	GLN A 173	30.522	18.729	13.061	1.00 26.34
MOTA	-	GLN A 173	30.783	19.753	13.345	1.00 26.57
MOTA		GLN A 173	31.252	20.872		1.00 23.68
MOTA		GLN A 173	30.492	19.386	11.822	1.00 25.00
MOTA	1289 N	GLN A 174	33.972	17.985	16.867	1.00 25.25
MOTA	1290 CA	GLN A 174	34.931	18.124	17.944	
MOTA	1291 C	GLN A 174	36.380	18.182	17.392	1.00 25.74
MOTA	1292 0	GLN A 174	37.152	19.066	17.767	1.00 24.76
MOTA	1293 CB	GLN A 174	34.770	16.951	18.923	1.00 25.13
MOTA	1294 CG	GLN A 174	35.771	16.925	20.048	1.00 26.00
MOTA	1295 CD	GLN A 174 .	35.636	15.697	20.929	1.00 26.76
ATOM	1296 OE1	GLN A 174	35.278	14.629	20.450	1.00 28.02
MOTA	1297 NE2	GLN A 174	35.917	15.851	22.222	1.00 26.75
ATOM	1298 N	GLY A 175	36.724	17.249	16.505	1.00 25.61
MOTA	1299 CA	GLY A 175	38.040	17.201	15.887	1.00 26.56
ATOM	1300 C	GLY A 175	38.333	18.393	14.980	1.00 27.62
ATOM	1301 0	GLY A 175	39.371	19.051	15.111	1.00 28.21
ATOM	1302 N	LYS A 176	37.415	18.695	14.074	1.00 28.41
ATOM	1303 CA	LYS A 176	37.583	19.834	13.173	1.00 29.52
ATOM	1304 C	LYS A 176	37.778	21.177	13.895	1.00 29.38
ATOM	1305 0	LYS A 176	38.557	22.009	13.443	1.00 29.30
MOTA	1306 CB	LYS A 176	36.371	19.977	12.257	1.00 29.90
ATOM	1307 CG	LYS A 176	36.212	18.895	11.227	1.00 32.69
ATOM	1308 CD	LYS A 176	35.023	19.242		1.00 36.10
ATOM	1309 CE	LYS A 176	34.114	18.065	10.148	1.00 37.89
ATOM	1310 NZ	LYS A 176	32.736		9.746	1.00 40.12
ATOM	1311 N	ARG A 177	37.060			1.00 29.00
ATOM	1312 CA	ARG A 177	37.164		15.710	1.00 29.17
ATOM	1313 C	ARG A 177	38.260		16.781	1.00 28.13
ATOM	1314 0	ARG A 177	38.433		17.394	1.00 27.46
ATOM	1315 CB	ARG A 177	35.831		16.391	1.00 29.67
ATOM	1316 CG	ARG A 177	34.600			1.00 31.86
MOTA	1317 CD	ARG A 177	34.629		14.243	1.00 35.68
	1317 CB		33.69			1.00 38.08
MOTA	1319 CZ		33.86			1.00 40.57
MOTA		1 ARG A 177	34.95			
MOTA		2 ARG A 177	32.92			
ATOM		GLY A 178	38.97			
MOTA	1322 N		40.01			
MOTA	1323 CA		39.46			
MOTA	1324 C	GLY A 178	40.17			
ATOM	1325 0	GLY A 178	38.19			
MOTA	1326 N	TRP A 179	38.19			
MOTA	1327 CA			_		
MOTA		TRP A 179	38.25			
MOTA			38.90			
MOTA			36.12			
MOTA			35.36			
MOTA	1332 CI	01 TRP A 179	35.83	0 23.42	J 13.116	, 1.00 20.00

								•	•				
ATOM	1333	CD2	TRP A	. 1	L79		33.985	22.140	19.825	1.00	24.35		C
ATOM	1334	NE1 '	TRP A	. 1	179		34.822	24.122	19.153	1.00	24.53		N
ATOM	1335		TRP A				33.676	23.355	19.167		24.34		С
ATOM	1336	-	TRP F				32.982	21.177	19.957		23.62		С
MOTA	1337				179		32.417	23.627	18.659		22.63		C
ATOM	1338		TRP A				31.726	21.454	19.442		24.07		C
MOTA	1339		TRP A				31.453	22.674	18.811		23.17		C N
MOTA	1340		GLY A				38.061	20.669 19.737	23.210 24.240		25.61		C
MOTA	1341		GLY A				38.471 37.428	18.634	24.240		25.44 26.09		C
MOTA MOTA	1342 1343		GLY A				36.592	18.432	23.491		26.60	•	Ö
ATOM	1344		GLN A				37.448	17.934	25.503		26.33		N
MOTA	1345		GLN A				36.561	16.806	25.708		26.77		c
ATOM	1346		GLN A				35.099	17.180	25.953		26.26		Č
ATOM	1347		GLN A				34.775	18.291	26.371		25.90		0
ATOM	1348		GLN Z				37.044	15.970	26.887		27.12		С
ATOM	1349		GLN Z				36.689	16.543	28.269	1.00	29.66		С
MOTA	1350	CD	GLN 2	A	181		36.917	15.533	29.388	1.00	33.17		С
MOTA	1351	OE1	GLN 3	Ą	181		38.055	15.295	29.791		35.52		0
MOTA	1352	NE2	GLN 2	V.	181	•	35.839	14.920	29.869		35.59		N
MOTA	1353	N	LEU 2				34.238	16.225	25.646		25.83		N
MOTA	1354	CA	LEU :			•	32.831	16.241	26.021		25.59		С
MOTA	1355	С	LEU .				32.850	16.162	27.543		24.45		С
MOTA	1356	0	LEU .				33.433	15.209	28.084		23.27		0
MOTA	1357	CB	LEU .				32.180	14.958	25.499		25.74		C C
ATOM	1358	CG	LEU .				30.666	14.790	25.403 25.676		28.29 27.13		C
ATOM ATOM	1359 1360		LEU LEU				30.276 29.928	13.328 15.671	26.303		30.64		C
MOTA	1361	N N	THR				32.288	17.158	28.239		23.24		N
ATOM	1362	CA	THR				32.256	17.110	29.699		22.37		C
ATOM	1363	C	THR				30.956	16.504	30.150		22.01		С
ATOM	1364	Ō	THR				30.907	15.867	31.186		21.99		0
ATOM	1365	CB	THR				32.395	18.504	30.371	1.00	22.62		С
ATOM	1366	OG1	THR	A	183		31.367	19.393	29.893	1.00	20.93		0
MOTA	1367	CG2	THR	A	183		33.707	19.154	30.013	1.00	22.33		С
MOTA	1368	N	SER	A	184		29.885	16.711	29.396		21.54	•	N
MOTA	1369	CA	SER				28.622	16.146	29.810		21.58		C
MOTA	1370	С	SER				27.498	16.381	28.866		21.50	•	C
MOTA	1371	0	SER				27.610	17.168	27.928		21.85		0 C
MOTA	1372	CB	SER				28.209	16.715 18.072	31.158 31.056		21.78	•	0
MOTA	1373 1374	OG N	SER ASN				27.856 26.416	15.667	29.134		23.20		N
ATOM ATOM	1374	N CA	ASN				25.167	15.807	28.427		22.40		c
ATOM	1376	C	ASN				24.104	16.059	29.459		22.16		Ċ
MOTA	1377		ASN				23.802	15.189			22.11		0
ATOM	1378	СВ	ASN				24.794	14.523	27.664		22.46		C
MOTA	1379	CG			185		25.798	14.174	26.604		23.64		С
MOTA	1380	OD1	ASN	Α	185		26.582	13.257	26.789	1.00	25.26		0
ATOM	1381	ND2	ASN	A	185		25.794	14.907	25.494		22.02		N
ATOM	1382	N	LEU	A	186		23.507	17.228	29.391		22.02		N
MOTA	1383	CA			186		22.461	17.600	30.319		22.34		C
MOTA	1384	С			186		21.114	17.251	29.707		22.21		С
ATOM	1385	0			186		20.808	17.623			22.59		0
MOTA	1386				186		22.519				22.36		C
ATOM	1387	CG			186		21.650		31.739		23.03		C
MOTA	1388		LEU				22.124	19.073 21.213	33.069 31.782		22.66 21.88		C
ATOM	1389 1390		LEU		187		21.636 20.307				0 22.39		N
MOTA MOTA	1390				187		18.949				0 21.93		C
MOTA	1391				187		18.089				0 21.94		Č
ATOM	1393				187		18.163				0 21.56		ō
011	1000	-		- +	,		_0.103						-

ATOM	1394	СВ	LEU	Α	187	18.525	14.883	30.604	1.00	21.36		С
ATOM	1395		LEU			17.037	14.555	30.489	1.00	22.46		С
ATOM	1396		LEU			16.550	14.530	29.038	1.00	22.25		С
ATOM	1397		LEU			16.783	13.200	31.154	1.00	22.25		С
ATOM	1398	N	LEU			17.301	18.028	29.826	1.00	21.68		N
ATOM	1399	CA	LEU			16.400	19.052	30.329		22.46		С
ATOM	1400	С	LEU			14.925	18.743	30.021		22.70		С
ATOM	1401	Ō	LEU			14.511	18.622	28:864		23.01		0
ATOM	1402	СВ	LEU			16.747	20.432	29.769	1.00	22.51		С
ATOM	1403	CG	LEU			18.166	20.932	29.998	1.00	24.09		С
ATOM	1404		LEU			18.916	20.996	28.697	1.00	26.99		С
MOTA	1405	CD2	LEU	Α	188	18.135	22.308	30.564	1.00	25.94		C
ATOM	1406	N	ILE			14.117	18.652	31.061	1.00	22.31	•	N
ATOM	1407	CA	ILE			12.721	18.383	30.851	1.00	22.23		С
ATOM	1408	С	ILE			11.959	19.459	31.554	1.00	22.43		С
MOTA	1409	0			189	12.045	19.599	32.773	1.00	22.44		0
MOTA	1410	CB	ILE			12.328	17.009	31.369	1.00	21.56		С
ATOM	1411		ILE			13.178	15.944	30.695	1.00	21.26		С
ATOM	1412	CG2	ILE	A	189	10.873	16.794	31.078	1.00	21.74	•	С
ATOM	1413	CD1	ILE	Α	189	12.851	14.481	31.136		22.52		С
ATOM	1414	N	GLY	Α	190	11.226	20.239	30.770	1.00	23.11		N
ATOM	1415	CA	GLY	Α	190	10.545	21.396	31.294	1.00	23.06		C
ATOM	1416	С	GLY	A	190	9.084	21.395	30.988		23.56		С
ATOM	1417	0	GLY	A	190	8.594	20.646	30.117		23.29		0
MOTA	1418	N			191	8.385	22.224	31.755		24.04		N
MOTA	1419	CA			191	6.980	22.468	31.542		24.73		С
MOTA	1420	C	MET	A	191 .	6.837	23.623	30.576		24.58		С
MOTA	1421	0			191	7.747	24.464	30.443		24.72		0
MOTA	1422	CB			191	6.301		32.860		25.52		C
ATOM	1423	CG			191	6.212		33.806		26.99		C
MOTA	1424	SD			191	5.710		35.447		30.62		S
ATOM	1425	CE			191	4.076		35.135		32.05		C
ATOM	1426	N			192	5.701		29.893		24.37		N
MOTA	1427	CA			192	5.407		28.940		24.51		C
MOTA	1428	C			192	5.468		29.628		24.20		C O
ATOM	1429	0			192	5.013		30.745		24.12		C
ATOM	1430	CB			192	4.029		28.342		24.59		C
ATOM	1431	CG			192	2.930		29.384		26.08 26.38		C
ATOM	1432	CD			192	1.590		28.830				0
ATOM	1433				192	1.530		27.676 29.562		27.04 25.46		o.
MOTA	1434				192	6.045				24.44		N
MOTA	1435 1436				193 193	6.153				24.21		Č
MOTA MOTA	1430				193	7.428				23.71		č
ATOM	1438				193	7.728				24.97		Ö
MOTA	1439				194	8.181				23.27		N
ATOM	1440				1 194	9.445				22.47		C
ATOM	1441				194	10.465				22.35		C
ATOM	1442				194	10.594				22.38		0
ATOM	1443				A 194	10.108				22.17		С
ATOM	1444				A 194	9.476				22.24		С
ATOM	1445				A 194	8.47				23.81		0
ATOM	1446				A 194	10.07				18.58		N
ATOM	1447				A 195	11.22				21.64		N .
ATOM	1448				A 195	12.26				21.41		С
ATOM	1449				A 195	13.569				20.40		С
ATOM	1450				A 195	. 13.60				20.03		0
ATOM	1451				A 195	11.88				21.72		С
ATOM	1452				A 195	13.03				21.84		С
ATOM	1453				A 195	10.62			1.00	23.61		C
ATOM	1454				A 196	14.64		30.813	1.00	19.77		N

MOTA	1455	CA	THR .	Α	196	15.980	29.917	31.376	1.00 20.37		С
MOTA	1456	С	THR .	Α	196	16.467	31.291	30.933	1.00 20.92		С
MOTA	1457	0	THR .	A	196	16.649	31.505	29.724	1.00 20.45		0
MOTA	1458`	CB	THR	A	196	16.882	28.865	30.793	1.00 19.87		С
MOTA	1459	OG1	THR			16.457	27.564	31.227	1.00 21.07		Ö
MOTA	1460	CG2	THR			18.273	29.043	31.340	1.00 20.00		C
MOTA	1461	N.	PRO			16.602	32.225	31.879	$1.00 \cdot 21.53$		N
MOTA	1462.	CA	PRO			16.997	33.609	31.572	1.00 22.24		. C
ATOM	1463	С	PRO			18.375	33.688	30.952	1.00 22.26		С
MOTA	1464	0	PRO			19.195	32.773	31.130	1.00 22.66		0
MOTA	1465	CB	PRO			16.998	34.305	32.934	1.00 22.51		С
MOTA	1466	CG	PRO			16.282	33.411	33.839	1.00 22.92		С
ATOM	1467	CD	PRO			16.367	32.028	33.312	1.00 21.85		С
ATOM	1468	N	ALA			18.606	34.776	30.234	1.00 21.54		N
ATOM .	1469	CA	ALA			19.821	34.976	29.486	1.00 21.47		C
ATOM	1470	C	ALA			21.110	34.764	30.282	1.00 21.22		С
ATOM	1471	0	ALA			21.298	35.310	31.386	1.00 20.56		0.
MOTA	1472	CB	ALA			19.809	36.397	28.891	1.00 21.92		C
ATOM	1473	N	HIS			22.023	34.020	29.683	1.00 21.01		N
MOTA	1474	CA	HIS			23.321	33.764	30.288	1.00 21.40		C
MOTA	1475	C	HIS			24.250	33.279	29.213	1.00 21.61		C
MOTA	1476	0	HIS			23.811	33.017	28.089	1.00 21.18		0
MOTA	1477 1478	CB CG	HIS HIS			23.217	32.669	31.338	1.00 21.05		C
MOTA						22.864 21.576	31.354 31.048	30.746	1.00 22.98		
ATOM ATOM	1479 1480	ND1	HIS			23.630	30.287	30.370 30.399	1.00 21.97 1.00 21.48		N C
ATOM	1481		HIS			21.558	29.838	29.838	1.00 21.48		C
MOTA	1482	NE2	HIS			22.791	29.368	29.821	1.00 24.36		N
MOTA	1483	N	TYR			25.538	33.177	29.555	1.00 24.30		. N
MOTA	1484	CA	TYR			26.531	32.597	28.654	1.00 22.56		C
ATOM	1485	C	TYR			27.234	31.448	29.380	1.00 22.96		č
ATOM	1486	Ö	TYR			27.293	31.430	30.612	1.00 22.90		Ö
ATOM	1487	СВ	TYR			27.528	33.610	28.129	1.00 22.56		Č
ATOM	1488	CG	TYR			28.492	34.228	29.145	1.00 23.02		C
ATOM	1489	CD1				29.731	33.671	29.385	1.00 22.79		Ċ
MOTA	1490	CD2				28.180	35.419	29.799	1.00 23.89		C
MOTA	1491	CE1				30.612	34.229	30.283	1.00 22.32		С
ATOM	1492	CE2	TYR	Α	200	29.062	35.991	30.722	1.00 22.06	•	С
MOTA	1493	CZ	TYR	A	200	30.277	35.402	30.947	1.00 22.13		· c
MOTA	1494	OH	TYR	A	200	31.163	35.957	31.843	1.00 20.46		0
MOTA	1495	N	ASP			27.723	30.467	28.619	1.00 23.11		N
MOTA	1496	CA	ASP			28.433	29.326	29.213	1.00 23.02		С
MOTA	1497	С			201	29.833	29.338	28.687	1.00 23.38		С
MOTA	1498	0			201	30.038	29.811	27.597	1.00 24.05		0
MOTA	1499	CB			201	27.776	28.012	28.829	1.00 22.85		С
MOTA	1500	CG			201	26.365	27.898	29.338	1.00 21.12		С
ATOM	1501		ASP			26.176	27.802	30.568	1.00 23.22		0
MOTA	1502		ASP			25.387	27.845	28.574	1.00 20.55		0
ATOM	1503	N			202		28.820	29.437	1.00 23.78		N
ATOM	1504	CA			202	32.184	28.782	28.950	1.00 25.14		C
MOTA	1505	C			202	32.524	27.467	28.269	1.00 24.96		C
MOTA	1506	0			202	33.657	27.001	28.394	1.00 26.76		0
ATOM	1507	CB			202	33.218	28.965	30.091	1.00 24.67		C
MOTA	1508	CG			202	33.017	30.199	30.941	1.00 27.79		C
MOTA	1509	CD OF1			202	34.089	30.312	32.025	1.00 30.13		C
MOTA MOTA	1510 1511		GLU			34.018	29.584	33.030	1.00 32.67		0
ATOM	1511	N N	GLU		202	35.010	31.114 26.818	31.844	1.00 29.05		O N
ATOM	1512	CA			203	31.547 31.804	25.624	27.653 26.874	1.00 24.30 1.00 23.24		N
ATOM	1513	CA			203	31.036	25.764	25.572	1.00 23.24		C
ATOM	1514	0			203	30.122	26.560	25.468	1.00 22.84		0
ATOM	1010	9	GTIN	^	200	۷0.1∠2	20.500	20.400	1.00 23.00		J

MOTA	1516	CB	GLN A	A 2	203	31.373	24.363	27.618	1.00 2	3.43		C
ATOM	1517		GLN A			32.256	24.031	28.826	1.00 2	3.66		С
ATOM	1518	CD	GLN A	A 2	203	32.061	22.612	29.354	1.00 2	25.58		С
MOTA	1519	OE1	GLN A	A 2	203 ·	31.915	21.661	28.582	1.00 2	27.85		0
ATOM	1520	NE2	GLN A	A 2	203	32.084	22.468	30.670	1.00 2	25.67		N
MOTA	1521	N	GLN A	A · 2	204	31.465	25.013	24.575	1.00 2			N
ATOM ·	1522	CA	GLN A	A 2	204	30.791	24.910	23.299	1.00 2	22.51		С
ATOM	1523	С	GLN A	A 2	204	29.626	23.980	23.504	1.00 2	21.70		C
ATOM	1524	0	GLN A	A 2	204	29.737	23.026	24.255	1.00 2	21.24		0
MOTA	1525	CB	GLN Z	A 2	204	31.718	24.307	22.255	1.00 2	22.29		C
MOTA	1526	CG	GLN Z	A 2	204	33.001	25.081	22.072	1.00 2	22.69		С
ATOM	1527	CD	GLN A	A 2	204	32.820	26.346	21.259	1.00 2	22.39		С
ATOM	1528	OE1	GLN I	A 2	204	31.699	26.736	20.932	1.00	19.22		0
MOTA	1529	NE2	GLN Z	A 2	204	33.937	26.970	20.906	1.00	19.77		N
ATOM	1530	N	ASN Z	A 2	205	28.523	24.241	22.810	1.00	21.48		N
MOTA	1531	CA	ASN .	A 2	205	27.309	23.471	23.017	1.00	21.04		С
MOTA	1532	С	ASN	A 2	205	26.558	23.136	21.730	1.00	21.10		С
MOTA	1533	0	ASN .	A 2	205	26.188	24.043	20.949	1.00	20.02		0
MOTA	1534	CB	ASN .	A :	205	26.401	24.322	23.920	1.00	21.70		C
MOTA	1535	CG	ASN .	A :	205	25.084	23.654	24.269	1.00	21.87		C
MOTA	1536	OD1	ASN .	A :	205	24.732	22.577	23.775	1.00			0
MOTA	1537	ND2	ASN	A :	205	2,4.332	24.320	25.118	1.00	19.37		N
ATOM	1538	N	PHE	A :	206	26.350	21.835	21.497	1.00			Ν.
ATOM	1539	CA	PHE	A :	206	25.372	21.414	20.523	1.00	20.14		С
MOTA	1540	C	PHE	Α	206	24.141	21.030	21.323		19.94		С
MOTA	1541	0	PHE	A.	206	24.164	20.052	22.065		20.71		0
MOTA	1542	CB	PHE	A	206	25.851	20.238	19.693		20.65		С
MOTA	1543	CG	PHE	Α	206	26.799	20.618	18.620	1.00	20.30		С
ATOM	1544	CD1	PHE	A	206	26.394	21.438	17.600		20.89		С
ATOM	1545	CD2	PHE	A	206	28.101		18.642		21.26		С
MOTA	1546		PHE			27.254		16.605		22.17	•	С
MOTA	1547	CE2	PHE			28.980		17.641		21.31		С
ATOM	1548	CZ	PHE	A	206	28.558	21.336	16.632		21.79		C ·
MOTA	1549	N	PHE			23.058		21.081		19.87		Ŋ
MOTA	1550	CA	PHE			21.790		21.824		20.08		С
MOTA	1551	С	PHE			20.766		20.975		20.29		С
ATOM	1552	0	PHE			20.276				19.94		0
ATOM	1553	CB	PHE			21.385				20.46		С
MOTA	1554	CG	PHE			20.129		22.890		19.14		C
MOTA	1555		PHE			18.947				19.77		C
MOTA	1556		PHE			20.169		24.259		19.99		C
ATOM	1557		·PHE			17.818				21.67		C
MOTA	1558		PHE			19.037		24.992		22.36		C
MOTA	1559	CZ	PHE			17.854				22.30		C
ATOM	1560	N	ALA			20.480				21.01		N
ATOM	1561	CA	ALA			19.688				21.26		C
MOTA	1562	С	ALA			18.260				21.74		C
MOTA	1563	0	ALA			18.000				21.21		0
ATOM	1564		ALA			20.365				20.94		C
ATOM	1565	N			209	17.329				21.56		N
ATOM	1566	CA			209	15.940				21.78	•	C
ATOM	1567	С			209	15.289				21.84		C
ATOM	1568	0			209	15.50				20.40		0
ATOM	1569		· GLN			15.20				22.08		C
ATOM	1570	CG			209	13.79				22.02	,	C
ATOM	1571	CD			209	13.68				22.84	•	C
ATOM	1572		GLN			14.70				22.55		0
ATOM	1573		2 GLN			12.44				21.97		N
MOTA	1574	N			210	14.48	•			22.17 22.53		N
ATOM	1575	CA			210	13.90				23.45		C
ATOM	1576	С	نظيا لـ	A	210	12.39	7 16.074	21.316	, T.OO	23.43		Ç

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MOTA	1577	0	ILE A		11.813	15.429	20.467	1.00 24.08	0
ATOM	1578	CB	ILE A		14.411	15.306	22.541	1.00 22.81	С
ATOM	1579				15.857	14.886	22.284	1.00 23.77	С
ATOM	1580	CG2	ILE A		13.573	14.064	22.785	1.00 23.17	C
ATOM	1581 1582	N	ILE A		16.631 11.772	14.512 16.778	23.519	1.00 24.86	C
ATOM ATOM	1583	CA	LYS A		10.318		22.258 22.351	1.00 23.73	N
ATOM	1584	.C	LYS A		9.873	18.253	22.566	1.00 22.99 1.00 22.73	C
ATOM	1585	0	LYS A		10.436	18.969	23.391	1.00 22.73	0
ATOM	1586	СВ	LYS A		9.818	16.014	23.527	1.00 23.40	C
ATOM	1587	CG	LYS A		8.285	15.757	23.509	1.00 24.55	Č
MOTA	1588	CD	LYS A		7.794	15.232	24.870	1.00 25.75	Č
ATOM	1589	CE	LYS A	211	6.389	14.579	24.861	1.00 25.61	С
MOTA	1590	NZ	LYS A	211	5.580	14.641	23.613	1.00 25.29	N
MOTA	1591	N	GLY A		8.832	18.655	21.847	1.00 22.34	N
ATOM	1592	CA	GLY A		8.292	19.989	21.983	1.00 22.46	С
ATOM	1593	С	GLY F		9.188	21.026	21.338	1.00 22.40	С
ATOM	1594	0	GLY A		10.172	20.705	20.650	1.00 21.93	0
ATOM	1595	N CA	TYR A		8.859	22.281	21.592	1.00 22.95	И
ATOM ATOM	1596 1597	CA C	TYR A		9.530 10.079	23.400	20.944	1.00 23.32	C
ATOM	1598	0	TYR A		9.434	24.412 24.740	21.926 22.918	1.00 23.27 1.00 23.34	C
ATOM	1599	СВ	TYR A		8.547	24.092	20.012	1.00 23.34	. С
ATOM	1600	CG	TYR A		8.133	23.198	18.887	1.00 25.58	č
ATOM	1601	CD1			. 7.110	22.261	19.041	1.00 28.74	C
MOTA	1602	CD2	TYR A	A 213	8.798	23.253	17.687	1.00 28.55	С
MOTA	1603	CE1	TYR A		6.764	21.410	17.995	1.00 30.77	C
MOTA	1604	CE2	TYR A		8.465	22.429	16.651	1.00 30.41	C
MOTA	1605	CZ		A 213	7.461	21.516	16.795	1.00 31.44	С
ATOM	1606	OH		A 213	7.188	20.720	15.708	1.00 35.50	0
ATOM	1607	N		A 214	11.270	24.911	21.620	1.00 22.60	N
ATOM ATOM	1608 1609	CA C		A 214 A 214	11.916 12.353	25.911	22.431	1.00 22.58	C
ATOM	1610	0		A 214	12.937	27.077 26.898	21.576 20.493	1.00 22.52 1.00 23.74	C 0
ATOM	1611	СВ		A 214	13.132	25.345	23.169	1.00 23.74	C
MOTA	1612	CG		A 214	12.784	24.539	24.392	1.00 22.79	· c
MOTA	1613	CD	LYS 2	A 214	14.053	24.007	25.077	1.00 22.96	C
MOTA	1614	CE	LYS 2	A 214	13.821	23.675	26.530	1.00 20.69	C
MOTA	1615	NZ		A 214	15.076	23.085	27.149	1.00 19.14	N
ATOM	1616	N		A 215	12.037	28.277	22.047	1.00 21.95	N
ATOM	1617		ARG		12.480	29.482	21.378	1.00 21.48	C
ATOM	1618	C		A 215	13.790	29.864	22.018	1.00 21.06	C
ATOM ATOM	1619 1620	O CB		A 215 A 215	13.890 11.466	29.954 30.582	23.230 21.576	1.00 20.53	0
ATOM	1621	CG		A 215	11.400		20.969	1.00 22.15 1.00 22.00	C
ATOM	1622	CD		A 215	11.231		21.727	1.00 23.87	c
ATOM	1623	NE		A 215	11.224	34.272	20.959	1.00 25.87	Ŋ
MOTA	1624	CZ		A 215	10.566		21.297	1.00 25.54	C
MOTA	1625		ARG I		9.873	35.425	22.423	1.00 24.05	N
ATOM	1626	NH2	ARG 2		10.634	36.420	20.505	1.00 29.37	N
ATOM	1627	N		A 216	. 14.794		21.193	1.00 21.48	N
MOTA	1628	CA		A 216	16.123		21.668	1.00 21.40	С
MOTA	1629	C		A 216	16.533		21.146	1.00 21.86	C
ATOM	1630	0		A 216	16.532		19.948	1.00 22.82	0
ATOM ATOM	1631 1632	CB SG		A 216	17.079 16.689		21.127	1.00 21.46	C
ATOM	1633	N N		A 216 A 217	16.878		21.469 22.045	1.00 22.63 1.00 21.29	S
ATOM	1634	CA		A 217	17.331		21.663	1.00 21.29	N C
ATOM	1635	C.		A 217	18.782		22.102	1.00 21.28	C
MOTA	1636	ō		A 217			23.310	1.00 20.00	0
ATOM	1637	СВ		A 217	16.456		22.327	1.00 21.80	č
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MOTA	1638	CG1 ILE A 217	14.978		21.955	1.00 22.90
ATOM	1639	CG2 ILE A 217	16.874		21.861	1.00 22.72
ATOM	1640	CD1 ILE A 217	14.031	35.695	22.693	1.00 24.99
ATOM	1641	N LEU A 218	19.666	34.346	21.128	1.00 20.25
ATOM	1642	CA LEU A 218	21.094	34.451	21.373	1.00 20.55
MOTA	1643	C LEU A 218	21.630	35.853	21.128	1.00 21.19
ATOM	1644	O LEU A 218	21.141	36.560	20.253	1.00 21.62
ATOM	1645	CB LEU A 218	21.874	33.493	20.467	1.00 20.31
ATOM	1646	CG LEU A 218	21.964	32.019	20.906	1.00 20.46
	1647	CD1 LEU A 218	20.628	31.415	21.054	1.00 20.19
MOTA		CD2 LEU A 218	22.732	31.229	19.907	1.00 22.84
ATOM	1648		22.658	36.231	21.886	1.00 21.06
ATOM	1649		23.331	37.498	21.682	1.00 21.62
ATOM	1650	CA PHE A 219		37.244	21.611	1.00 21.87
ATOM	1651	C PHE A 219	24.842	36.490	22.416	1.00 21.88
ATOM	1652	O PHE A 219	25.390		22.410	1.00 20.94
ATOM	1653	CB PHE A 219	23.005	38.484		1.00 20.34
ATOM	1654	CG PHE A 219	21.541	38.617	23.106	
MOTA	1655	CD1 PHE A 219	20.907	37,779	23.995	1.00 21.92
ATOM	1656	CD2 PHE A 219	20.785	39.589	22.476	1.00 24.21
MOTA	1657	CE1 PHE A 219	19.563	37.915	24.250	1.00 21.95
ATOM .	1658	CE2 PHE A 219	19.442	39.724	22.735	1.00 22.06
MOTA	1659	CZ PHE A 219	18.840	38.904	23.621	1.00 23.11
MOTA	1660	N PRO A 220	25.512	37.877	20.662	1.00 22.38
MOTA	1661	CA PRO A 220	26.962	37.744	20.557	1.00 22.81
MOTA	1662	C PRO A 220	27.683	38.287	21.793	1.00 22.78
ATOM	1663	O PRO A 220	27.173	39.123	22.564	1.00 22.88
MOTA	1664	CB PRO A 220	27.335	38.561	19.317	1.00 22.81
ATOM	1665	CG PRO A 220	26.005	39.005	18.685	1.00 23.68
ATOM	1666	CD PRO A 220	24.940	38.792	19.663	1.00 22.86
ATOM	1667	N. PRO A 221	28.885	37.774	21.999	1.00 22.84
ATOM	1668	CA PRO A 221	29.724	38.204	23.124	1.00 22.73
ATOM	1669	C PRO A 221	29.976	39.714	23.143	1.00 22.28
ATOM	1670	O PRO A 221	30.192	40.279	24.212	1.00 21.03
	1671	CB PRO A 221	31.030	37.455	22.892	1.00 22.78
MOTA	1672	CG PRO A 221	30.644	36.296	22.026	1.00 23.22
MOTA		CD PRO A 221	29.521	36.733	21.174	1.00 22.58
ATOM	1673	· · · · · · · · · · · · · · · · · · ·	29.897	40.378	21.993	1.00 22.60
ATOM	1674		30.172	41.821	21.965	1.00 22.84
MOTA	1675		28.996		22.493	
ATOM	1676		29.031			
MOTA	1677				20.579	
MOTA	1678		30.638	42.389	19.537	
ATOM	1679		29.502		19.764	
MOTA	1680		28.355			
ATOM	1681		29.690			
ATOM	1682		27.940			
ATOM	1683		26.826			
MOTA	1684		26.942			
MOTA	1685		25.986			
ATOM	1686		25.510			
MOTA	1687		25.217			
MOTA	1688		23.786			
ATOM	1689		22.861			
MOTA	1690		23.592			
ATOM	1691		28.111			
ATOM	1692	2 CA, PHE A 224	28.394			
ATOM	1693		27.888			
ATOM	1694		27.233			
MOTA	1695		29.917	7 42.068		
ATOM	1696		30.309			
MOTA	1697		30.449			
MOTA	1698		30.583		3 29.27	9 1.00 20.92

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MOTA	1699	CE1	PHE A	224	30.842	42.945	30.868	1.00 2	2.58		С
ATOM	1700		PHE A		30.979	40.593	30.587	1.00 2			С
ATOM	1701	CZ	PHE A		31.087	41.725	31.394	1.00 2			С
MOTA	1702	N	GLU A		28.190	44.665	27.106	1.00 2			N
ATOM	1703	CA	GLU A		27.813	45.963	27.677	1.00 2			С
MOTA	1704	С	GLU A		26.322	46.216	27.764	1.00 2			С
ATOM	1705	0	GLU A		25.907	47.129	28.483	1.00 2			0
ATOM	1706	CB	GLU A		28.396	47.111	26.856	1.00 2			С
ATCM	1707 1708	CG CD	GLU A		29.897 30.386	47.228 48.632	27.013 27.280	1.00 3 1.00 3			C C
MOTA MOTA	1708		GLU A		29.901	49.319	28.242	1.00 3			0
ATOM	1710		GLU A		31.310	49.028	26.532	1.00 4			0
MOTA	1711	N	CYS A		25.532	45.456	27.003	1.00 4			N
ATOM	1712	CA	CYS A		24.087	45.619	27.027	1.00 2			C
ATOM		.C	CYS A		23.372	44.631	27.935	1.00 2			Č
ATOM	1714	Ō	CYS A		22.170	44.781	28.162	1.00 2			ō
ATOM	1715	ĊВ	CYS A		23.523	45.416	25.630	1.00 2			C
MOTA	1716	SG	CYS A		24.206	46.488	24.368	1.00 2			S
MOTA	1717	N	LEU A		24.102	43.633	28.451	1.00 2		-	N
MOTA	1718	CA	LEU A		23.467	42.529	29.169	1.00 2	22.08		С
ATOM	1719	С	LEU A	. 227	23.771	42.393	30.657	1.00 2	21.99		С
ATOM	1720	0	LEU · A	. 227	23.118	41.611	31.373	1.00 2	22.28		0
MOTA	1721	CB	LEU A	. 227	23.751	41.244	28.418	1.00 2	22.29		C
ATOM	1722	CG	LEU A		22.874·	41.185	27.158	1.00 2	23.54		С
ATOM			LEU A		23.428	40.186	26.144	1.00 2			С
ATOM			LEU A		21.423	40.819	27.5.44	1.00 2			С
ATOM		N	TYR A		24.763	43.140	31.109	1.00 2			N.
MOTA		CA	TYR A		24.996	43.320	32.521	1.00 2			С
ATOM		C	TÝR A		25.018	42.057	33.382	1.00			C
ATOM		0	TYR A		24.205	41.920	34.301	1.00			0
MOTA		CB	TYR A		23.957	44.311	33.077	1.00			C C
MOTA MOTA		CG CD1	TYR A		·23.949 24.768	45.649 46.677	32.339 32.739	1.00			C
ATOM		CD2			23.122	45.862	31.232	1.00			C
ATOM		CE1			24.780	47.912	32.076	1.00			C
ATOM		CE2			23.117	47.074	30.561	1.00			C
ATOM		CZ	TYR A		23.931	48.113	31.000	1.00			Ċ
ATOM		OH	TYR A		23.947	49.325	30.336	1.00			ō
MOTA		N	PRO A		25.985	41.175	33.141.				N
ATOM		CA	PRO A	•	26.128	39.971	33.966	1.00			С
ATOM	1739	С	PRO P	229	26.428	40.332	35.408	1.00	20.08		C
ATOM	1740	0	PRO A	229	27.021	41.379	35.675	1.00	20.20		0
MOTA	1741	CB	PRO P	A 229	27.360	39.271	33.363	1.00	20.51		С
MOTA		CG	PRO F		28.084	40.340	32.651	1.00			С
MOTA		CD	PRO P		27.025	41.241	32.105	1.00			С
ATOM		N	TYR A		25.988	39.490	36.326	1.00			N
ATOM		CA	TYR A		26.282	39.656	37.724	1.00			С
ATOM		C	TYR F		27.809	39.657	37.947	1.00			С
ATOM		0	TYR A		28.575	39.250	37.094	1.00			0
ATOM		CB	TYR A		25.669	38.507	38.520	1.00			C
ATOM		CG	TYR A		24.172	38.597	38.725		19.28		C
ATOM			TYR		23.297	38.110	37.760		18.53		C
ATOM ATOM			TYR A		23.629	39.172	39.885		19.38		C
ATOM			TYR A		21.932 22.234	38.161 39.222	37.935 40.076		18.86		C
ATOM		CEZ		A 230	21.404	38.719	39.073		19.53 20.93		C
ATOM		OH		A 230	20.034	38.771	39.176		23.69		0
ATOM		N		A 231	28.251	40.137	39.098		18.40		N
ATOM		CA		A 231	29.651	39.983	39.476		18.58		C
ATOM		C		A 231	30.070	38.507	39.399		19.41		C
ATOM		ō		A 231		37.624	39.654		18.89		ŏ
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ATOM	1760	CB	PRO A 231	29.675	40.477	40.931	1.00 18.95		С
ATOM	1761	CG	PRO A 231	28.542	41.507	41.001	1.00 19.02		C
ATOM	1762	CD	PRO A 231	27.460	40.868	40.105	1.00 18.02		С
ATOM	1763	N	VAL A 232	31.335	38.248	39.071	1.00 19.55		N
ATOM	1764	CA	VAL A 232	31.826	36.884	38.969	1.00 20.65		С
	1765	C	VAL A 232	31:640	36.034	40.236	1.00 20.79		C
ATOM		0	VAL A 232	31.379	34.838	40.145	1.00 21.82		Ö
ATOM	1766			33.318	36.869	38.545	1.00 20.71		Ċ
ATOM	1767	CB.			35.524	38.807	1.00 20.71		Ċ
ATOM	1768		VAL A 232	33.945					C
ATOM	1769		VAL A 232	33.452	37.225	37.075	1.00 20.83		
MOTA	1770	N	HIS A 233	31.770	36.639	41.409	1.00 20.87		N
MOTA	1771	CA	HIS A 233	31.643	35.907	42.661	1.00 20.70		C
MOTA	1772	С	HIS A 233	30.203	35.739	43.168	1.00 20.59		C
MOTA	1773	0	HIS A 233	29.940	35.010	44:119	1.00 20.49		0
ATOM	1774	CB	HIS A 233	32.482	36.593	43.706	1.00 20.63		С
ATOM	1775	CG	HIS A 233	33.948	36.529	43.426	1.00 21.92		C
ATOM	1776	ND1	HIS A 233	34.659	37.595	42.913	1.00 22.17		N
MOTA	1777		HIS A 233	34.843	35.527	43.610	1.00 22.03	•	С
ATOM	1778		HIS A 233	35.929	37.249	42.793	1.00 23.69		С
ATOM	1779		HIS A 233	36.066	35.998	43.203	1.00 23.04		N
MOTA	1780	N	HIS A 234	29.273	36.433	42.543	1.00 20.53		N
	1781	CA	HIS A 234	27.869	36.251	42.857	1.00 20.60		C
MOTA			HIS A 234	27.388	34.895	42.306	1.00 20.45		Ċ
ATOM	1782	C			34.428	41.291	1.00 19.86		Õ
MOTA	1783	0	HIS A 234	27.873		42.206	1.00 19.00		Ċ
MOTA	1784	CB	HIS A 234	27.088	37.359		1.00 20.63		C
ATOM	1785	CG	HIS A 234	25.661	37.441	42.625			
ATOM	1786		. HIS A 234	24.667	36.700	42.021	1.00 21.46		И
ATOM	1787		HIS A 234	25.044	38.249	43.518	1.00 20.20		C
MOTA	1788		. HIS A 234	23.504	37.013	42.563	1.00 21.99		C
MOTA	1789	NE2	2 HIS A 234	23.707	37.951	43.473	1.00 21.29		N
MOTA	1790	N	PRO A 235	26.463	34.261	43.007	1.00 20.40		N
ATOM	1791	CA	PRO A 235	25.888	32.993	42.572	1.00 20.85		С
ATOM	1792	С	PRO A 235	25.360	33.021	41.152	1.00 21.20		С
ATOM	1793	.0	PRO A 235	.25.437	31.984	40.502	1.00 20.43		0
ATOM	1794	СВ	PRO A 235	24.756	32.771	43.575	. 1.00 21.58		С
ATOM	1795	CG	PRO A 235	25.273		44.826	1.00 20.78		С
ATOM	1796	CD	PRO A 235	25.941		44.317	1.00 20.56		С
ATOM	1797	N	CYS A 236	24.905		40.663	1.00 20.46		N
ATOM	1798	CA	CYS A 236	24.379		39.308	1.00 20.63		C
	1799	C	CYS A 236	25.430		38.301			Č
ATOM			CYS A 236	25.110		37.258	1.00 21.60		ō
MOTA	1800	0				39.268	1.00 20.06		č
ATOM	1801	CB	CYS A 236	23.114					S
ATOM	1802	SG	CYS A 236	21.824					N
ATOM	1803		ASP A 237						C
ATOM	1804			27.785				•	. C
MOTA	1805		ASP A 237	27.381					
ATOM	1806		ASP A 237	26.830					0
MOTA	1807								C
ATOM	1808	CG	ASP A 237						C
ATOM	1809	OD	1 ASP A 237	30.407	35.010	36.546			0
MOTA	1810		2 ASP A 237						0
MOTA	1811	N	ARG A 238	27.664	34.812	35.263	1.00 20.18		N
MOTA	1812						1.00 21.48		С
ATOM	1813		ARG A 238						С
ATOM	1814		ARG A 238						0
ATOM	1815								Č
									, C
ATOM	1816								C
MOTA	1817								N
ATOM	1818								C
MOTA	1819								
MOTA	1820) NH	11 ARG A 23	27.20	8 29.799	32.90	1.00 24.08		N

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ATOM	1821		ARG A		27.399	28.949	35.036	1.00 2	7.47	N
ATOM	1822		GLN A		25.021	35.028	34.375	1.00 2		N
MOTA	1823		GLN A		23.641	35.334	34.014	1.00 2		С
ATOM	1824		GLN A		23.459	36.865	33.920	1.00 2		С
MOTA	1825		GLN A		24.145	37.624	34.610	1.00 2		0
ATOM	1826		GLN A.		22.646	34.776	35.027	1.00 2		C
ATOM	1827		GLN A		23.052	33.505	35.726	1.00 2		C
MOTA	1828		GLN A		23.281	32.320	34.807	1.00 2		C
MOTA	1829		GLN A		22.367	31.842	34.132	1.00 2		0
ATOM	1830		GLN A		24.502	31.834 37.307	34.796 33.071	1.00 2		N N
MOTA	1831	N CA	SER A SER A		22.541 22.246	38.725	32.926	1.00 2		C
ATOM ATOM	1832	CA	SER A		21.448	39.218	34.119	1.00 2		C
ATOM	1833 1834	0	SER A		20.538	38.533	34.564	1.00 2		0
ATOM	1835	СВ	SER A		21.384	38.953	31.700	1.00		Ċ
ATOM	1836	OG	SER A		21.018	40.312	31.564	1.00 2		.0
ATOM	1837	N	GLN A		21.763	40.408	34.623	1.00		N
ATOM	1838	CA	GLN A		20.962	40.988	35.701	1.00		C
ATOM	1839	C	GLN A		19.657	41.569	35.175	1.00		Č
ATOM	1840	ō	GLN A		18.808	41.956	35.959	1.00		Ö
ATOM	1841	СВ	GLN A		21.697	42.141	36.417	1.00		C
ATOM	1842	CG	GLN A		22.910	41.749	37.230	1.00	21.41	С
ATOM	1843	CD	GLN A	241	23.690	42.980	37.695	1.00	22.76	C
MOTA	1844		GLN A		23.455	43.481	38.775	1.00	24.42	0
ATOM	1845	NE2	GLN A	241	24.585	43.465	36.871	1.00	21.93	N
MOTA	1846	N	VAL A	242	19.489	41.678	33.862	1.00	20.66	N
MOTA	1847	CA	VAL A	242	18.309	42.355	33.372	1.00	20.76	С
MOTA	1848	С	VAL A	242	17.089	41.465	33.391		21.26	С
MOTA	1849	0	VAL A		17.119	40.352	32.871		21.01	0
MOTA	1850	CB	VAL A		18.476	42.813	31.909		20.97	C
MOTA	1851		VAL A		17.194	43.502	31.431		21.21	C
MOTA	1852		VAL A		19.687	43.704	31.716		18.95	C
ATOM	1853	N	ASP A		16.001	41.960	33.958		21.16	N
ATOM	1854	CA	ASP A		14.730	41.223	33.907		21.36	C
MOTA	1855	C	ASP A		14.091	41.523	32.552		21.20	C
MOTA	1856	0	ASP A		13.566	42.631	32.310		19.97	0
ATOM	1857	CB	ASP A		13.840	41.682	35.054		21.65	C
MOTA	1858	CG	ASP A		12.474	41.051	35.037		22.45	0
ATOM	1859		ASP A ASP A		12.122 11.671	40.338 41.232	34.070 35.978		25.16 25.29	0
ATOM' ATOM	1860 1861	N N	PHE A		14.182	40.554	31.650		21.28	N
ATOM	1862	CA	PHE A		13.687	40.733	30.291		21.65	C
ATOM	1863	C	PHE A		12.202	41.074	30.274		22.36	c
ATOM	1864	Ö	PHE A		11.733	41.653	29.304		22.09	Ö
ATOM	1865	СB	PHE A		13.915	39.478			22.22	Ċ.
ATOM	1866	CG	PHE A		15.284	39.370			21.43	Ċ
ATOM	1867		PHE A		16.414	39.800			20.12	C
MOTA	1868		PHE A		15.422	38.778			21.05	C
MOTA	1869		PHE A		17.655	.39.671			20.83	С
MOTA	1870		PHE A		16.645	38.643			21.47	С
MOTA	1871	CZ	PHE A		17.767	39.104	27.633	1.00	20.74	С
MOTA	1872	N	ASP A	245	11.464	40.696	31.322	1.00	23.26	N
MOTA	1873	CA	ASP A	245	10.035	40.973	31.393	1.00	24.31	С
MOTA	1874	С	ASP A		9.756				25.05	С
MOTA	1875	0	ASP A	245	8.679				24.27	0
MOTA	1876	СВ	ASP A		9.333				24.79	C
MOTA	1877	CG	ASP A		9.397				25.46	С
MOTA	1878		ASP A		9.409				27.47	0
MOTA	1879		ASP A		9.445				25.22	0
MOTA	1880	N	ASN A		10.702				25.30	N
MOTA	1881	CA	ASN A	246	10.531	44.365	33.099	1.00	26.37	Ċ

MOTA	1882	C F	ASN A	246	11.876	45.054		1.00 25.61	C
ATOM	1883	_	A NEA		12.436	45.192		1.00 26.05	0
MOTA	1884		ASN A		9.871	44.360		1.00 26.89	C
ATOM	1885		ASN A		9.545	45.770		1.00 30.93	C
MOTA	1886		A NR		9.353	46.701		1.00 35.10	0
MOTA	1887		ASN A		9.493	45.943	36.281	1.00 35.04	N N
MOTA	1888		PRO A		12.415	45.450	32.068 32.026	1.00 24.71 1.00 24.24	C
·ATOM	1889		PRO A		13.775	45.979 47.352	32.684	1.00 24.24	Č
MOTA	1890		PRO A		13.909 13.189	48.296	32.374	1.00 24.40	Ö
MOTA	1891		PRO A PRO A		14.109	46.036	30.538	1.00 24.23	Č
ATOM	1892		PRO A		12.900	45.524	29.803	1.00 25.13	Č
ATOM	1893		PRO A		11.769	45.385	30.752	1.00 24.61	C.
ATOM	1894 1895		ASP A		14.867	47.437	33.593	1.00 24.04	N
ATOM ATOM	1896		ASP A		15.140	48.656	34.285	1.00 24.53	С
ATOM	1897		ASP A		16.206	49.440	33.496	1.00 24.15	C
ATOM	1898		ASP A		17.410	49.221	33.629	1.00 23.11	0
ATOM	1899		ASP A		15.609	48.312	35.689	1.00 24.75	С
ATOM	1900		ASP A		15.731	49.512	36.554	1.00 26.08	С
ATOM	1901		ASP A		15.956	50.616	36.009	1.00 27.08	0
MOTA	1902	OD2	ASP A	248	15.623	49.439	37.797	1.00 30.33	0
MOTA	1903	N	TYR A	. 249	15.735	50.329	32.642	1.00 24.42	N
MOTA	1904	CA	TYR A	249	16.612	51.129	31.807	1.00 25.30	C
MOTA	1905	С	TYR F	249	17.462	52.136	32.589	1.00 26.13	C
MOTA	1906		TYR F		18.495	52.584	32.083	1.00 26.46	0
MOTA	1907		TYR A		15.796	51.826	30.713	1.00 25.41	C
MOTA	1908	CG	TYR A		15.119	50.853	29.768	1.00 22.90	C
MOTA	1909		TYR A		15.844	49.873	29.130	1.00 22.91	C
MOTA	1910	CD2	TYR A		13.760	50.923	29.519	1.00 22.21 1.00 22.19	c
MOTA	1911	CE1		A 249	15.238	48.964	28.271 28.660	1.00 22.19	Ċ
MOTA	1912	CE2		A 249	13.144	50.023	28.046	1.00 21.30	C
MOTA	1913	CZ		A 249	13.895 13.304	49.044 48.163	27.173	1.00 23.38	ō
ATOM	1914 1915	OH		A 249 A 250	17.071	52.465	33.822	1.00 26.65	N
ATOM	1915	N CA		A 250	17.894	53.365	34.640	1.00 27.47	С
ATOM ATOM	1917	C		A 250	19.161	52.651	35.086	1.00 26.52	C
ATOM	1918	Ö		A 250	20.238	53:224	35.086	1.00 27.17	0
ATOM	1919	СВ		A 250	17.133	53.908	35.866	1.00 27.89	С
ATOM	1920	CG		A 250	15.880	54.684	35.485	1.00 32.57	С
ATOM	1921	CD		A 250	15.258	55.459	36.631	1.00 37.09	
ATOM	1922	OE1	GLU	A 250	15.809	55.491	37.753	1.00 42.28	
MOTA	1923	OE2		A 250	14.198	56.055	36.399	1.00 42.29	
MOTA	1924	N	ARG	A 251	19.042	51.399	35.490	1.00 25.57	
MOTA	1925	CA		A 251	20.224	50.657	35.900	1.00 24.72	
MOTA	1926	C		A 251	20.955	50.069		1.00 23.56	
MOTA	1927	0		A 251	22.150	49.919		1.00 22.92	
ATOM	1928	СВ		A 251	19.845	49.520		1.00 25.64 1.00 26.79	
MOTA	1929			A 251	19.435	49.957		1.00 20.79	
MOTA	1930			A 251	18.858			1.00 30.01	
ATOM	1931			A 251	19.900 19.709				
ATOM	1932			A 251	18.508				
ATOM	1933 1934			A 251 A 251	20.734				
MOTA	1934			A 251	20.734				
MOTA	1935			A 252	20.234			•	
ATOM ATOM	1930			A 252	20.521				
ATOM	1938			A 252	19.900				
ATOM	1939			A 252	20.261				
ATOM	1940			A 252	20.292				5 C
MOTA	1941			A 252	21.484			1.00 20.90	0 C
ATOM	1942			A 252	19.124				4 C
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ATOM	1943		PHE A			21.506	46.040		1.00 20.51	C	
ATOM	1944		PHE A			19.136	45.730	35.662	1.00 21.77	C	
ATOM	1945	CZ	PHE A			20.320	45.553	36.333	1.00 21.41	(
MOTA	1946 1947	N CA	PRO I			20.989	50.944	31.071	1.00 20.88	1	
MOTA MOTA	1947	CA	PRO A			20.615 20.956	51.754	29.909	1.00 20.51		2
ATOM	1949	0	PRO I			20.356	51.077 51.159	28.578	1.00 20.47 1.00 20.01	()
ATOM	1950	СВ	PRO I			21.371	53.077	30.130	1.00 20.01) C
ATOM	1951	CG	PRO I			22.538	52.697	31.136	1.00 20.46		ت ت
ATOM	1952	CD	PRO I			21.921	51.641	31.994	1.00 20.40		J. C
MOTA	1953	N	ASN Z			22.088	50.393	28.455	1.00 20.68		N
ATOM	1954	CA	ASN Z			22.401	49.805	27.160	1.00 20.72		C
ATOM'	1955	С	ASN 2	Α	254	21.537	48.601	26:790	1.00 20.29		С
MOTA	1956	0	ASN Z	Α	254	21.644	48.068	25.688	1.00 20.03		0
MOTA	1957	CB	ASN 2		•	23.882	49.463	27.033	1.00 20.89		С
MOTA	1958	CG	ASN A			24.736	50.698	26.899	1.00 22.24		C
MOTA	1959		ASN .			25.532	50.999	27.785	1.00 24.48		0
ATOM	1960		ASN 2			24.557	51.446	25.791	1.00 22.23		N
ATOM	1961 1962	N CA	PHE .			20.678	48.160	27.690	1.00 20.01		N
ATOM ATOM	1962	CA	PHE .			19.781 18.855	47.086 47.599	27.305 26.185	1.00 20.02		C
ATOM	1964	0	PHE .			18.224	46.818	25.472	1.00 20.33 1.00 19.82		С 0
ATOM	1965	CB	PHE			18.970	46.552	28.484	1.00 19.63		c
ATOM	1966	CG	PHE .			18.239	45.318	28.145	1.00 18.96		C
ATOM	1967		PHE			18.928	44.149	27.930			C
MOTA	1968		PHE			16.889	45.335	27.942	1.00 17.83		C
ATOM	1969	CE1	PHE			18.267	42.997	27.575			С
MOTA	1970	CE2	PHE			16.230	44.206	27.561			С
MOTA	1971	CZ	PHE			16.912	43.036	27.381			С
MOTA	1972	N	GLN			18.788	48.919	26.035			N
ATOM	1973	CA	GLN		•	17.973	49.533	24.986			С
ATOM	1974	С	GLN			18.594	49.343	23.591			C
ATOM ATOM	1975 1976	O CB	GLN GLN			17.955	49.612	22.592			0
ATOM	1977	CG	GLN			17.787 16.744	51.036 51.306	25.272 26.362			C
ATOM	1978	CD	GLN			16.747	52.732	26.888			C
ATOM	1979	OE1	GLN			15.727	53.420	26.816			Ö
MOTA	1980	NE2				17.873	53.172	27.419			N
ATOM	1981	N	ASN	Α	257	19.850	48.915	23.553			N
MOTA	1982	CA	ASN	A	257	20.583	48.700	22.310	1.00 20.66		С
MOTA	1983	С	ASN	Α	257	20.778	47.233	21.963	1.00 21.21		С
MOTA	1984	0	ASN			21.446	46.921	20.979			0
MOTA	1985	CB	ASN			21.975	49.300	22.420			С
ATOM	1986	CG	ASN			21.937	50.757	22.776			C
ATOM ATOM	1987 1988		ASN ASN			22.395	51.141	23.850			0
ATOM	1988	N N	VAL			21.366	51.577	21.889			N
ATOM	1990	CA	VAL			20.218 20.440	46.333 44.908	22.758 22.532			N C
ATOM	1991	C	VAL			19.720	44.400	21.284			C
ATOM	1992	ō			258	18.600	44.845	20.947			o
ATOM	1993	CB			258	20.026	44.110	23.772			C
MOTA	1994		VAL			18.529	43.868	23.785			Ċ
MOTA	1995		VAL			20.761	42.851	23.826			С
MOTA	1996	N			. 259	20.381	43.506	20.562	2 1.00 24.48		N
MOTA	1997	CA			259	19.787	42.922	19.364	1.00 25.21		С
MOTA	1998	С			259	20.104	41.427	19.331			С
ATOM	1999	0			259	21.260	41.046	19.333			0
ATOM	2000	CB			259	20.345	43.551	18.094			C
ATOM ATOM	2001 2002		VAL			19.726	42.893	16.882			C
ATOM .	2002	N	VAL		259	20.074 19.068	45.059 40.603	18.066			C
MION	2003	IN	311	А	. 400	13.000	40.003	19.308	3 1.00 25.20	,	N

ATOM	2004	CA	GLY A 2	60	19.214	39.161	19.312	1.00 2		C
MOTA	2005 ·	С	GLY A 2	60	19.108	38.433	17.961	1.00 2		C
MOTA	2006	0	GLY A 2	60	18.762	39.016	16.914	1.00 2		0
MOTA	2007	N	TYR A 2	61	19.484	37.160	18.015	1.00		N
ATOM	2008	CA	TYR A 2		19.379	36.217	16.925	1.00		C
MOTA	2009	С	TÝR A 2		18.435	35.145	17.475	1.00		С
MOTA	2010	0	TYR A 2	61	18.671	34.620	18.552	1.00		0
ATOM	2011	CB	TYR A 2	61	20.730	35.574	16.627	1.00		С
MOTA	2012	CG	TYR A 2	261	21.748	36.476	15.965	1.00		С
MOTA	2013	CD1	TYR A 2	61	21.804	36.598	14.585	1.00		С
ATOM	2014	CD2	TYR A 2	261	22.649	37.194	16.712	1.00		С.
ATOM	2015	CE1	TYR A 2	261	22.737	37.429	13.976	1.00		С
MOTA	2016	CE2	TYR A 2	261	23.592	37.994	16.126	1.00		C
MOTA	2017	CZ	TYR A 2	261	23.643	38.116	14.768	1.00		C
MOTA	2018	OH	TYR A 2	261	24.580	38.959	14.202	1.00		0
MOTA	2019	N	GLU A 2	262	17.353	34.823	16.790	1.00		N
MOTA	2020	CA	GLU A 2	262	16.432	33.860	17.387		23.96	С
ATOM	2021	С	GLU A 2	262	15.992	32.773	16.435	1.00	23.90	С
ATOM	2022	0	GLU A 2	262	16.116	32.890	15.213	1.00	23.56	0
MOTA	2023	CB	GLU A 2	262	15.224	34.553	18.020	1.00	23.70	C
MOTA	2024	CG	GLU A 2	262	14.029	34.782	17.127	1.00	24.33	C
ATOM	2025	CD	GLU A	262	12.829	35.382	17.870	1.00	26.49	· c
ATOM	2026	OE1	GLU A		12.753	36.611	18.029	1.00	27.38	0
ATOM	2027	OE2	GLU A	262	11.946	34.631	18.306	1.00	28.26	0
ATOM	2028	N	THR A		15.485	31.713	17.034	1.00	23.68	N
ATOM	2029	CA	THR A		14.974	30.605	16.279	1.00	24.40	C
ATOM	2030	С	THR A		14.091	29.786	17.193	1.00	24.29	C
ATOM	2031	0	THR A		14.131	29.936	18.423	1.00	24.53	0
ATOM	2032	CB	THR A		16.148	29.762	15.751	1.00	24.52	C
ATOM	2033	OG1			15.684	28.839	14.762	1.00	24.43	0
ATOM	2034	CG2			16.737	28.876	16.854	1.00	24.33	,C
MOTA	2035	N	VAL A		13.263	28.954	16.593	1.00	23.62	N
ATOM	2036	CA	VAL A		12.500	28.019	17.370	1.00	24.01	С
ATOM	2037	С	VAL A		12.936	26.627	16.935	1.00	24.53	С
ATOM	2038	0	VAL A		12.879	26.291	15.768	1.00	24.27	0
ATOM	2039	СВ	VAL A		11.008	28.194	17.177	1.00	24.69	C
ATOM	2040		VAL A		10.256	26.958	17.712	1.00	23.69	C
ATOM	2041		VAL A		10.520	29.526	17.857	1.00	23.81	C
ATOM	2042	N	VAL A		13.450	25.844	17.872	1.00	24.91	N
MOTA	2043	CA.	VAL A		13.833	24.484	17.540	1.00	24.93	С
ATOM	2044	C	VAL A		12.792	23.,470	17.967	1.00	24.20	С
MOTA	2045	0	VAL A	265	12.167	23.617	19.018	1.00	24.01	0
MOTA	2046	CB	VAL A		15.196	24.072	18.173	1.00	25.05	С
ATOM	2047	CG1	VAL A		16.291	24.884	17.557	1.00	26.38	С
MOTA	2048	CG2	VAL A	265 ·	15.190	24.164	19.702	1.00	23.59	С
MOTA	2049	N	GLY A		12.641	22.439	17.144	1.00	23.26	N
MOTA	2050	CA	GLY A		11.776	21.316	17.451	1.00	23.22	С
MOTA	2051	С	GLY A	266	12.467	19.961	17.359	1.00	22.26	C.
ATOM	2052	0	GLY A		13.661	19.872	17.131	1.00	22.37	0
ATOM	2053	N	PRO A		11.712	18.884	17.524	1.00	21.90	N
ATOM	2054	CA	PRO A	267	12.305	17.544	17.479	1.00	21.60	C
ATOM	2055	С	PRO A		13.206		16.280	1.00	20.82	C
ATOM	2056		PRO A		12.768				20.29	0
ATOM	2057		PRO A		11.086				21.36	С
MOTA	2058		PRO A		10.023				23.23	С
ATOM	2059		PRO A		10.254				21.99	С
ATOM	2060		GLY A		14.445				20.81	N
ATOM	2061		GLY A		15.340				20.31	С
ATOM	2062		GLY A		16.296				20.37	С
ATOM	2063		GLY A		17.333				21.79	0
ATOM	2064		ASP A		15.975				19.89	N
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ATOM	2065	CA	ASP	A	269	16.849	20.141	15.364	1.00 19.78		С
MOTA	2066	С	ASP	Α	269	17.991	20.162	16.395	1.00 19.63		Ċ
MOTA	2067	0	ASP	Α	269	17.829	19.729	17.551	1.00 18.28		0
MOTA	2068	CB	ASP	Α	269	16.069	21.436	15.532	1.00 20.34		C
MOTA	2069	CG	ASP	Α	269	14.976	21.636	14.500	1.00 20.66		С
MOTA	2070	OD1	ASP	A	·269	14.977	21.015	13.419	1.00 22.15	•	0
MOTA	2071	OD2	ASP			14.072	22.454	14.703	1.00 23.30		0
ATOM	2072	N	VAL	Α	270	19.129	20.681	15.953	1.00 19.76		N
MCTA	2073	CA			270	20.304	20.879	16.782	1.00 20.24		C
ATOM	2074	C			270	20.793	22.318	16.601	1.00 19.84		С
ATOM	2075	0	VAL			21.052	22.754	15.487	1.00 19.90		0
ATOM	2076	,CB			270	21.421	19.942	16.377	1.00 20.08		С
MOTA	2077		VAL			22.676	20.288	17.121	100 21.38		C
ATOM	2078		VAL			21.017	18.521	16.671	1.00 21.15		С
MOTA	2079	N	LEU			20.885	23.056	17699	1.00 19.86		N
ATOM	2080	CA			271	21.341	24.427	17.656	1.00 20.03		С
ATOM	2081	C			271	22.757	24.465	18.202	1.00 20.23	•	C
ATOM	2082	0			271	23.032	23.946	19.276	1.00 19.73		0
MOTA	2083	CB			271	20.429	25.328	18.465	1.00 20.59		С
ATOM	2084	CG			271	20.934	26.742	18.724	1.00 20.93		C
ATOM	2085	CD1				21.011	27.562	17.431	1.00 20.35		С
ATOM	2086		LEU			20.039	27.428	19.728	1.00 22.31		С
MOTA	2087	N			272	23.669	25.024	17.416	1.00 20.58		N
ATOM	2088	CA			272	25.010	25.229	17.883	1.00 20.58		С
ATOM	2089	С			272	24.985	26.535	18.653	1.00 20.69	_	C
ATOM ATOM	2090	O			272	24.692	27.576	18.089	1.00 21.54	•	0
ATOM	2091 2092	CB CG			272	26.004	25.312	16.728	1.00 20.30		C
ATOM	2092	CD1			272	27.381	25.776	17.158	1.00 21.24		C
ATOM	2093	CD2			272	27.997	25.250	18.275	1.00 21.70		С
ATOM	2095		TYR			28.039	26.788	16.472	1.00 22.21		C
ATOM	2096		TYR			29.232 29.275	25.692	18.674	1.00 21.69		C
ATOM	2097	CZ			272	29.868	27.215 26.672	16.857 17.961	1.00 22.99		C
ATOM	2098	ОН			272	31.109	27.111	18.352	1.00 22.01 1.00 22.77		C
ATOM	2099	N			273	25.216	26.454	19.951	1.00 22.77		O N
ATOM	2100	CA			273	25.362	27.629	20.805	1.00 21.22		C
ATOM	2101	C			273	26.852	27.809	21.117	1.00 21.49		C
ATOM	2102	Ō			273	27.413	27.112	21,962	1.00 22.55		Õ
MOTA	2103	CB			273	24.607	27.471	22.073	1.00 21.14		Ċ
ATOM	2104	CG1			273	23.148	27.132	21.776	1.00 21.68		C
MOTA	2105	CG2	ILE			24.661	28.791	22.854	1.00 21.75		Č
MOTA	2106		ILE			22.318	26.972	23.026	1.00 21.44		c
ATOM	2107	N			274	27.493	28.723	20.413	1.00 21.86		N
MOTA	2108	CA			274	28.929	28.916	20.557	1.00 22.49		C
ATOM	2109	С	PRO	Α	274	29.278	29.462	21.926	1.00 22.77		C
MOTA	2110	0	PRO	Α	274	28.510	30.231	22.521	1.00 21.72		0
MOTA	2111	CB	PRO	A	274	29.305	29.908	19.429	1.00 23.00		С
ATOM	2112	CG	PRO	Α	274	28.022	30.225	18.658	1.00 23.03		С
MOTA	2113	CD			274	26.889	29.582	19.398	1.00 22.21		С
ATOM	2114	N			275	30.441	29.028	22.404	1.00 22.72		N
MOTA	2115	CA			275	30.962	29.403	23.702	1.00 23.40		С
ATOM	2116	C			275	30.949	30.921	23.864	1.00 22.42		С
ATOM	2117	0			275	31.282	31.636	22.937	1.00 20.73		0
MOTA	2118	CB			275	32.373	28.856	23.826	1.00 23.99		С
MOTA	2119	CG			275	32.933	28.944	25.203	1.00 28.99		С
ATOM	2120	SD			275	34.517	28.083	25.337	1.00 35.05		S
MOTA	2121	CE			275	35.287	28.525	23.832	1.00 31.30		С
ATOM	2122	N			276	30.509	31.388	25.030	1.00 22.30		N
ATOM	2123	CA			276	30.419	32.831	25.349	1.00 23.06		С
ATOM	2124	C			276	29.221	33.543	24.752	1.00 22.11		С
ATOM	2125	0	TYR	. A	276	29.012	34.705	25.041	1.00 21.84		0

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ATOM	2126 CE					1.00 23.42	C
MOTA	2127 CG					1.00 28.51	C
ATOM	2128 CD	1 TYR A 276				1.00 33.00	C
ATOM	2129 CI	2 TYR A 276	33.876			1.00 34.41	С
ATOM	2130 CE	E1 TYR A 276	34.066	33.490		1.00 36.36	С
ATOM		E2 TYR A 276	34.968	32.151		1.00 36.45	С
ATOM	2132 C2		35.059	32.651	27.371	1.00 37.63	С
ATOM	2133 OF			32.314	28.077	1.00 40.88	0
ATOM	2134 N		28.455	32.878	23.906	1.00 20.75	N
ATOM	2135 C		27.272	33.528	23.360	1.00 20.85	. C
MOTA	2136 C	TRP A 277	26.173	33.482		1.00 20.33	С
	2137 0		25.907	32.431		1.00 20.72	0
ATOM			26.791	32.874	22.068	1.00 20.13	С
ATOM			27.552	33.323	20.879	1.00 19.28	С
MOTA			28.887	33.175	20.673	1.00 21.27	С
MOTA		D1 TRP A 277	27.042	33.995	19.730	1.00 20.60	Ċ
MOTA		D2 TRP A 277		33.721	19.467	1.00 21.05	N
MOTA		E1 TRP A 277	29.246			1.00 21.03	. C
MOTA		E2 TRP A 277	28.128	34.232	18.864	1.00 21.04	C
MOTA		E3 TRP A 277	25.780	34.456	19.352		C
MOTA		Z2 TRP A 277	. 27.989	34.893	17.643	1.00 20.38	. C
MOTA		Z3 TRP A 277		35.110	18.122	1.00 20.48	
MOTA	2147 C	H2 TRP A 277	26.736	35.306	17.288	1.00 21.03	C
MOTA	2148 N	TRP A 278	25.572	34.632	24.629	1.00 19.39	N
MOTA	2149 C	A TRP A 278	24.430	34.711	25.521	1.00 19.80	C
ATOM	2150 C	TRP A 278	23.243	33.927	24.927	1.00 20.18	C
ATOM	2151 O		23.019	33.939	23.732	1.00 21.04	0
ATOM		B TRP A 278	23.989	36.168	25.646	1.00 20.39	С
ATOM		G TRP A 278	24.979	37.031	26.300	1.00 21.20	С
ATOM		D1 TRP A 278	26.022	37.672	25.720	1.00 21.06	С
ATOM		D2 TRP A 278	25.056	37.301	27.691	1.00 20.38	C
ATOM		NE1 TRP A 278	26.725	38.369	26.668	1.00 22.44	N
ATOM		CE2 TRP A 278	26.139	38.155	27.891	1.00 21.86	С
MOTA		CE3 TRP A 278	24.282	36.937	28.789	1.00 21.09	С
ATOM		CZ2 TRP A 278	26.480	38.640	29.147	1.00 21.13	С
ATOM		CZ3 TRP A 278	24.623	37.412	30.019	1.00 23.38	С
		CH2 TRP A 278	25.704	38.258	30.194	1.00 21.06	С
ATOM		N HIS A 279	22.465	33.278	25.761	1.00 20.76	N
ATOM		CA HIS A 279	21.262	32.646	25.294	1.00 21.56	С
ATOM			20.198	32.659	26.361	1.00 21.24	С
ATOM			20.130		27.540	1.00 21.63	Ō
ATOM		O HIS A 279	21.501	31.203	24.819	1.00 21.83	, c
MOTA		CB HIS A 279		30.379	25.738	1.00 23.50	Ċ
MOTA		CG HIS A 279	22.342	30.494	25.785	1.00 24.98	Ŋ
MOTA		ND1 HIS A 279	23.713		26.602	1.00 24.30	C
MOTA		CD2 HIS A 279	22.017	29.385 29.599		1.00 26.21	Ċ
MOTA		CE1 HIS A 279	24.200			1.00 25.14	N
ATOM		NE2 HIS A 279	23.192	28.927		1.00 23.14	N
MOTA		N HIS A 280	18.994	32.900			C
MOTA		CA HIS A 280	17.736			1.00 21.78	c
MOTA		C HIS A 280	16.890			1.00 21.70	
ATOM	2175	O HIS A 280	16.722			1.00 21.40	0
MOTA		CB HIS A 280	17.104			1.00 21.20	C
MOTA		CG HIS A 280					C
ATOM		ND1 HIS A 280					N
ATOM	2179	CD2 HIS A 280					C
MOTA	2180	CE1 HIS A 280					C
ATOM		NE2 HIS A 280					N
ATOM		N ILE A 281	16.368				N
ATOM		CA ILE A 281		29.779			
MOTA		C ILE A 281					
ATOM		O ILE A 281					
ATOM		CB ILE A 281			26.301	1.00 23.87	С
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MOTA	2187		ILE			17.771	28.675	25.435	1.00 25.77	С
ATOM	2188		ILE			15.748	27.261	25.863	1.00 23.54	C
MOTA	2189		ILE			18.752	27.659	25.690	1.00 29.36	С
MOTA	2190	N	GLU			13.268	29.510	25.982	1.00 23.92	N
MOTA	2191	CA	GLU			11.923	29.337	26.525	1.00 24.26	C .
MOTA	2192	C	GLU			11.113	28.234	25.834	1.00 23.82	C
ATOM	2193	0	GLU			11.115	28.107	24.606	1.00 24.00	0
MOTA	2194	CB	GLU			11.166	30.681	26.490	1.00 24.35	C
ATOM ATOM	2195 2196	CG CD	GĻU GLU			10.887 10.320	31.249 32.668	25.112 25.168	1.00 25.59	C
ATOM	2197	OE1	GLU			10.861	33.494	25.100	1.00 25.45 1.00 26.04	0
ATOM	2198	OE2	GLU			9.332	32.954	24.451	1.00 25.04	0
ATOM	2199	N	SER			10.460	27.419	26.648	1.00 23.28	N
ATOM	2200	CA	SER			9.573	26.373	26.166	1.00 23.66	c
ATOM	2201	C	SER			8.257	27.054	25.787	1.00 23.86	Ċ
ATOM	2202	0	SER			7.678	27.780	26.593	1.00 23.20	Ō
ATOM	2203	CB	SER			9.341	25.321	27.247	1.00 23.36	C
MOTA	2204	OG	SER	Α	283	10.473	24.497	27.401	1.00 23.30	0
MOTA	2205	N	LEU	A	284	7.792	26.837	24.564	1.00 24.56	N
MOTA	2206	CA	LEU			6.626	27.583	24.084	1.00 25.62	C
MOTA	2207	С	LEU			5.401	27.487		1.00 25.52	C
MOTA	2208	0	LEU			5.114	26.431	25.589	1.00 24.71	0
MOTA	2209	CB	LEU			6.237	27.157	22.680	1.00 25.64	С
ATOM	2210	CG	LEU			7.274	27.308	21.576	1.00 27.12	С
MOTA	2211		LEU			6.591	27.546	20.242	1.00 28.93	C
ATOM	2212		LEU			8.248	28.364	21.851	1.00 27.08	С
MOTA	2213	N			285	4.713	28.615	25.144	1.00 25.85	N
MOTA	2214	CA			285	3.490	28.676	25.942	1.00 26.84	C
ATOM	2215	C			285	2.507	27.691	25.345	1.00 27.10	C
ATOM	2216	O			285	2.424	27.565	24.139	1.00 27:10	0
ATOM ATOM	2217 2218	CB CG			285 285	2.875 3.709	30.071	25.906	1.00 26.48	C
ATOM	2219	CD1			285	3.709	31.225 32.554	26.438 26.026	1.00 27.70 1.00 28.22	C
ATOM	2220		LEU			3.845	31.125	27.928	1.00 28.22	C
ATOM	2221	N			286	1.779	26.987	26.196	1.00 27.81	N
ATOM	2222	CA			286	0.790	26.007	25.753	1.00 28.27	C
ATOM	2223	C			286	1.313	24.977	24.744	1.00 27.42	C
MOTA	2224	Ō			286	0.555	24.481	23.922	1.00 26.50	ō
MOTA	2225	CB			286	-0.417	26.741	25.160	1.00 29.08	C
MOTA	2226	CG			286	-0.931	27.846	26.078	1.00 32.15	C
MOTA	2227	OD1			286	-1.484	27.577	27.154	1.00 34.93	0
ATOM	2228	ND2	ASN	A	286	-0.725	29.099	25.670	1.00 35.91	N
ATOM	2229	N			287	2.608	24.672	24.799	1.00 26.54	N
MOTA	2230	CA			287	3.201	23.727	23.879	1.00 25.64	C
MOTA	2231	С			287	3.474	22.371	24.497	1.00 25.01	С
MOTA	2232	0			287	4.031	21.502	23.829	1.00 24.77	0
ATOM	2233	N			288	3.110	22.187	25.766	1.00 24.43	N
ATOM	2234	CA			288	3.357	20.922	26.455	1.00 23.99	С
ATOM	2235	C			288	4.804	20.844	26.935	1.00 24.11	C
ATOM	2236	0			288	5.546		26.786	1.00 22.82	0
ATOM	2237	N			289	5.211		27.472	1.00 23.99	N
ATOM	2238	CA			289	6.550		28.000	1.00 24.69	C
ATOM	2239	C			289	7.605		26.908	1.00 24.25	C
ATOM ATOM	2240 2241	O CB			289	7.350 6.691		25.774 28.836	1.00 25.20 1.00 25.39	0
ATOM	2241				289	6.702		27.941	1.00 25.39	C
ATOM	2242				289	5.613		29.921	1.00 27.43	.C
ATOM	2244				289	7.255		28.650	1.00 20.30	C
ATOM	2245	N			290	8.808		27.267	1.00 30.37	N
ATOM	2246	CA			290	9.908		26.334	1.00 23.28	C
ATOM	2247	C			290	11.008		26.824	1.00 21.52	č
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MOTA	2248		THR A			1.193	18.789	28.029	1.00 2			0
ATOM	2249		THR A			0.473	21.318	26.168	1.00 2			C
MOTA	2250	OG1	THR A	. 290		0.758	21.885	27.444	1.00 2			0
MOTA	2251	CG2 '	THR A	. 290		9.436	22.268	25.557	1.00 2			C
ATOM	2252		ILE A			1.746	18.421	25.880	1.00 2			N
ATOM	2253		ILE A		1	2.880	17.616	26.234	1.00 2			С
ATOM	2254	C	ILE A	291 -	1	4.033	17.981	25.347	1.00 2			С
ATOM	2255	0	ILE A	291		3.869	18.064	24.137	1.00 2			0
ATOM .	2256		ILE A		1	2.559	16.118	26.078	1.00 2			С
ATOM	2257		ILE A		1	1.405	15.724	27.004	1.00 2			С
ATOM	2258	CG2	ILE A	291	1	3.798	15.310	26.383	1.00 2			C
ATOM	2259	CD1	ILE A	291	1	0.969	14.262	26.867	1.00 2			C
ATOM	2260	N	THR P	A 292		5.194	18.188	25.953	1.00 2			N
MOTA	2261	CA	THR P	A 292		6.395	18.517	25.236	1.00 2			С
ATOM	2262	С	THR A	A 292	1	7.560	17.794	25.831	1.00 2			С
ATOM	2263	0	THR A	A 292	1	7.605	17.557	27.021	1.00 2			0
MOTA	2264	CB	THR A	A 292	1	6.688	20.044	25.365	1.00 2			С
ATOM	2265	OG1	THR A	A 292	1	5.524	20.799	25.022	1.00	19.08		0
ATOM	2266	CG2	THR A	A 292]	.7.730	20.487	24.355	1.00 2			С
ATOM	2267	N	VAL A	A 293	1	8.530	17.454	25.003	1.00	20.52		N
ATOM	2268	CA	VAL A	A 293	1	19.784	16.939	25.516	1.00	20:48		С
ATOM	2269	С	VAL 2	A 293	2	20.892	17.803	24.918	1.00	20.80		С
MOTA	2270	0	VAL A	A 293	2	20.936	17.954	23.709	1.00	19.58	•	0
ATOM	2271	CB	VAL A	A 293		19.995	15.483	25.129	1.00	20.78		С
ATOM	2272	CG1		A 293	:	21.436	15.068	25.385	1.00	20.33		С
ATOM	2273			A 293	:	19.047	14.597	25.919	1.00	20.95		C
ATOM	2274	N		A 294		21.749	18.412	25.752	1.00	21.34		N
ATOM	2275	CA	ASN I	A 294		22.855	19.192	25.205	1.00	22.04		С
ATOM	2276	С		A 294		24.144	18.362	25.204	1.00	22.29		C
ATOM	2277	Ō		A 294		24.182	17.241	25.720	1.00	23.22		0
ATOM	2278	CB		A 294		23.012	20.581	25.883	1.00	22.35		С
ATOM	2279	CG		A 294		23.703	20.520	27.259	1.00	23.08		С
MOTA	2280			A 294		24.240	19.493	27.628	1.00	22.91		0
ATOM	2281			A 294		23.657	21.640	28.027	1.00	21.75		N
ATOM	2282	N		A 295		25.168	18.903	24.565	1.00	22.27		N
ATOM	2283	CA		A 295		26.467	18.269	24.452	1.00	22.31		С
ATOM	2284	С		A 295		27.444	19.408	24.704	1.00.	22.66		С
ATOM	2285	0		A 295		27.602	20.299	23.865	1.00	23.12		0
ATOM	2286	СВ		A 295		26.709	17.748	23.040	1.00	22.32		С
ATOM	2287	CG		A 295		25.871	16.568	22.653	1.00	22.18		С
ATOM	2288			A 295		24.494	16.689	22.477	1.00	22.38		C
ATOM	2289	CD2	PHE	A 295	٠.	26.465	15.336	22.441	1.00	21.44	•	С
ATOM	2290			A 295		23.757	15.604		1.00	24.06		С
ATOM	2291			A 295		25.718	14.248	22.064	1.00	19.77		С
ATOM	2292	CZ		A 295		24.380	14.366	21.911	1.00	21.39		С
ATOM	2293	N		A 296		28.062	19.403	25.869	1.00	22.66	•	N
MOTA	2294	CA		A 296		28.998	20.450	26.256	1.00	23.09		С
ATOM	2295	С		A 296		30.454	19.991		1.00	23.22		С
ATOM	2296	Ō		A 296		30.865				22.78		0
ATOM	2297	СВ		A 296		28.734				22.89		С
ATOM	2298	CG		A 296		27.830				23.61		С
ATOM	2299			A 296		27.783				25.47		С
ATOM	2300			A 296		26.894				24.55		С
MOTA	2301			A 296		26.874				25.25		N
MOTA	2302			A 296		26.308				24.33		С
ATOM	2303			A 296		26.464				27.49		С
ATOM	2304			A 296		25.335				25.91		С
ATOM	2305			A 296		25.474				27.19		С
ATOM	2306			A 296		24.935				26.96		С
ATOM	2300			A 297		31.216				23.29		N
ATOM	2308			A 297		32.627				23.80		C
AION	2300	CA	7 7 1/	251								-

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ATOM	2309	С	TYR	A	297	33.506	21.660	25.554	1.00 24.51	С
ATOM	2310	0	TYR	A	297	33.188	22.825	25.323	1.00 23.73	0
ATOM	2311	CB	TYR			32.882	20.332	23.610	1.00 23.38	C
MOTA	2312	CG	TYR	Α	297	32.284	19.092	23.021	1.00 23.42	С
ATOM	2313	CD1	TYR	A	297	30.940	19.053	22.641	1.00 23.90	С
MOTA	2314	CD2	TYR	Α	·297	33.056	17.971	22.808	1.00 21.43	С
MOTA.	2315	CE1				30.394	17.920	22.089	1.00 23.32	С
ATOM	2316	CE2	TYR	Α	297	32.515	16.826	22.250	1.00 22.05	С
MOTA	2317	CZ	TYR			31.186	16.806	21.905	1.00 21.88	С
ATOM	2318	OH	TYR	Α	297	30.644	15.669	21.365	1.00 21.30	0
ATOM	2319	N			298 -	34.637	21.334	26.160	1.00 25.35	N
ATOM	2320	CA	LYS			35.589	22.362	26.536	1.00 26.48	C
ATOM	2321	С	LYS			36.070	23.017	25.268	1.00 26.23	C
ATOM	2322	0	LYS			36.224	22.364	24.249	1.00 24.85	0
ATOM	2323	ĊВ	LYS	Α	298	36.783	21.771	27.308	1.00 27.15	C
ATOM	2324	CG	LYS			36.474	21.471	28.777	1.00 30.00	C
ATOM	2325	CD	LYS			37.666	20.901	29.550	1.00 33.20	С
ATOM	2326	CE	LYS			37.232	20.493	30.969	1.00 36.09	C
ATOM	2327	NZ	LYS			38.299	19.766	31.764	1.00 39.03	N
MOTA	2328	N	GLY			36.321	24.313	25.329	1.00 27.13	N
ATOM	2329	CA	GLY			36.798	25.014	24.159	1.00 28.27	С
ATOM	2330	С			299	38.229	24.649	23.837	1.00 29.23	С
ATOM	2331	0	GLY			38.892	24.005	24.613	1.00 28.19	0
ATOM	2332	N			300 ·	38.674	25.046	22.660	1.00 31.78	N
ATOM	2333	CA	ALA			40.046	24.852	22.233	1.00 34.32	С
ATOM	2334	C ·	ALA			40.992	25.610	23.155	1.00 36.37	С
ATOM	2335	0	ALA			40.573	26.430	23.956	1.00 35.96	0
ATOM	2336	СВ	ALA			40.210	25.355	20.806	1.00 34.38	С
ATOM	2337	N	PRO			42.280	25.349	23.025	1.00 39.70	N
ATOM	2338	CA	PRO			43.278	26.051	23.845	1.00 41.64	С
ATOM	2339	C	PRO			43.465	27.482	23.386	1.00 43.35	C
ATOM	2340	0	PRO			43.220	27.803	22.228	1.00 43.86	0
ATOM ATOM	2341	CB	PRO			44.566	25.275	23.572	1.00 41.46	C
ATOM	2342 2343	CG CD	PRO			44.382	24.736	22.199	1.00 41.25	C
ATOM	2343	N	PRO			42.906	24.416	22.068	1.00 40.04	C
ATOM	2344	CA			302	43.900	28.328	24.300	1.00 45.97	N
ATOM	2345	CA			302 302	44.214	29.715	24.001	1.00 47.77	C
ATOM	2347	0.			302	45.593 46.532	29.713 29.251	23.362	1.00 48.92	C
ATOM	2348	CB			302	44.282	30.469	24.006 25.322	1.00 49.23	0
ATOM	2349	OG1				43.006	30.416	25.976	1.00 48.10	C
ATOM	2350		THR			44.520	31.924	25.100	1.00 49.37 1.00 48.91	_
ATOM	2351	N			303	45.761	30.248	22.148	1.00 48.91	C N
ATOM	2352	CA			303	47.064	30.150	21.474	1.00 50.62	C
MOTA	2353	C			303	48.191	30.728	22.316	1.00 50.64	C
MOTA	2354	Ο.			303	47.883	31.390	23.307	1.00 50.98	Ö
MOTA	2355	СВ			303	46.877	30.986	20.202	1.00 50.93	C
MOTA	2356	CG			303	45.407	30.999	19.968	1.00 50.70	Ċ
MOTA	2357	CD			303	44.814	31.064	21.360	1.00 50.45	Č
ATOM	2358	N			307	46.978	37.074	18.830	1.00 53.59	N
MOTA	2359	CA			307	46.946	38.016	17.714	1.00 53.82	Ĉ
MOTA	2360	С			307	45.902	39.090	17.922	1.00 52.97	c
MOTA	2361	0			307	44.792	38.810	18.358	1.00 53.64	ŏ
MOTA	2362	CB			307	46.672	37.308	16.371	1.00 54.37	Č
MOTA	2363	CG			307	46.875	38.231	15.159	1.00 56.16	c
MOTA	2364	CD			307	46.966	37.504	13.822	1.00 57.96	Ċ
MOTA	2365	OE1	GLU	A	307	46.621	36.303	13.738	1.00 59.31	ō
MOTA	2366	OE2			307	47.388	38.150	12.839	1.00 59.69	Ō
MOTA	2367	N			308	46.267	40.324	17.610	1.00 51.95	ทั
ATOM	2368	CA			308	45.343	41.436	17.702	1.00 51.19	C
ATOM	2369	С	TYR	Α	308	44.693	41.603	16.337	1.00 50.27	С

					1	00 50 45
ATOM	2370	O TYR A 308	45.246			1.00 50.45
ATOM	2371	CB TYR A 308	46.083			1.00 51.43
ATOM	2372	CG TYR A 308 ·	46.675	42.460	19.532	1.00 52.65
		CD1 TYR A 308	45.925	42.712		1.00 52.95
MOTA	2373			41.912		1.00 53.42
MOTA	2374	CD2 TYR A 308	47.948	41.312		
MOTA	2375	CE1 TYR A 308	46.435	42.472		1.00 54.01
ATOM	2376	CE2 TYR A 308	48.467	41.662		1.00 54.33
MOTA	2377	CZ TYR A 308	47.703	41.949		1.00 54.84
MOTA	2378	OH TYR A 308	48.189	41.714	23.323	1.00 56.45
	2379	N PRO A 309	43.496	42.186	16.290	1.00 48.69
MOTA			. 42.789	42.696		1.00 47.07
MOTA	2380	CA PRO A 309				1.00 44.55
MOTA	2381	C PRO A 309	42.127	41.586		
MOTA	2382	O PRO A 309	41.782	40.555		1.00 45.01
ATOM	2383	CB PRO A 309	41.720	43.606		1.00 47.45
ATOM	2384	CG PRO A 309	41.420	42.978		1.00 48.43
ATOM	2385	CD PRO A 309	42.701	42.336	15.056	1.00 48.78
	2386	N LEU A 310	41.967	41.790	19.577	1.00 41.78
ATOM			41.344	40.781		1.00 39.59
MOTA	2387			40.652	20.133	1.00 37.52
MOTA	2388	C LEU A 310	39.858			
MOTA	2389	O LEU A 310	39.171	41.655	19.923	1.00 38.11
MOTA	2390	CB LEU A 310	41.499	41.174	21.893	1.00 39.43
ATOM	2391	CG LEU A 310	42.527	40.468	22.784	1.00 38.86
ATOM	2392	CD1 LEU A 310	43.799	40.123	22.092	1.00 37.07
	2393	CD2 LEU A 310	42.799	41.326	24.000	1.00 38.37
MOTA			39.361	39.425	20.141	1.00 34.45
MOTA	2394	N LYS A 311			20.001	1.00 32.51
MOTA	2395	CA LYS A 311	37.932	39.180		1.00 32.51
MOTA	2396	C LYS A 311	37.144	39.537	21.257	
ATOM	2397	O LYS A 311	37.675	39.546	22.375	1.00 28.88
MOTA	2398	CB LYS A 311	37.674	37.736	19.652	1.00 32.87
ATOM	2399	N ALA A 312	35.853	39.786	21.057	1.00 28.39
ATOM	2400	CA ALA A 312	34.991		22.155	1.00 27.14
			35.110		23.260	1.00 26.12
ATOM	2401				24.411	1.00 24.47
ATOM	2402	O ALA A 312	35.274			1.00 26.63
. ATOM	2403	CB ALA A 312	33.552		21.710	
MOTA	2404	N HIS A 313	35.126		22.910	1.00 25.90
MOTA	2405	CA HIS A 313	35.106		23.932	1.00 25.82
ATOM	2406	C HIS A 313	36.411	36.749	24.690	1.00 25.03 [.]
ATOM	2407		36.447	36.323	25.825	1.00 24.89
	2408		34.724			1.00 27.19
MOTA			35.788			1.00 29.47
MOTA	2409					1.00 34.94
MOTA	2410		35.963			
MOTA	2411		36.753			
MOTA	2412	CE1 HIS A 313	37.006			1.00 35.11
MOTA	2413	NE2 HIS A 313	37.499			1.00 35.57
MOTA	2414		37.491	L 37.185	24.072	1.00 24.60
ATOM	2415		38.764		. 24.753	1.00 24.57
	2416		38.77			1.00 24.74
MOTA			39.37			1.00 24.48
MOTA	2417					1.00 24.79
MOTA	2418		39.89			
MOTA	2419		40.06			
ATOM	2420	O CD GLN A 314	41.10	9 36.488		
MOTA	2421		41.01	3 37.450	20.949	
ATOM	2422		42.12		21.699	1.00 29.52
	2423		38.11			
ATOM			37.98			
MOTA	2424					
MOTA	2425		37.09			
MOTA	2420		37.34			
ATOM	242	7 CB LYS A 315	37.40			
ATOM			38.40	3 42.449		
ATOM			37.82		3 24.226	1.00 34.17
MOTA			38.84			
AION	243	110 11 010	23.3.			

ATOM	2431	NZ	LYS A 315	38.206	45.270	22.318	1.00 41.38	N
ATOM	2432	N	VAL A 316	36.079	39.314	27.330	1.00 23.78	N
ATOM	2433	CA	VAL A 316	35.258	38.796	28.396	1.00 23.67	Č
ATOM	2434	С	VAL A 316	36.138	37.937	29.329	1.00 23.61	C
ATOM	2435	0	VAL A 316	36.094	38.075	30.558	1.00 22.63	0
ATOM	2436	CB	VAL A 316	34.092	37.961	27.873	1.00 23.67	C
ATOM	2437	CG1	VAL A 316	33.315	37.370	29.037	1.00 23.53	С
ATOM	2438	CG2	VAL A 316	33.159	38.816	27.005	1.00 23.69	С
MCTA	2439	N	ALA A 317	36.940	37.065	28.732	1.00 22.51	N
ATOM	2440	CA	ALA A 317	37.834	36.207	29.507	1.00 22.28	С
ATOM	2441	С	ALA A 317	38.7,30	37.067	30.391	1.00 21.32	С
ATOM	2442	0	ALA A 317	38.926	36.783	31.556	1.00 21.45	0
MOTA	2443	CB	ALA A 317	.38.680	35.325	28.574	1.00 21.87	С
MOTA	2444	N	ILE A 318	39.220	38.153	29.834	1.00 20.92	N
ATOM	2445	CA	ILE A 318	40.091	39.053	30.574	1.00 21.36	С
ATOM	2446	С	ILE A 318	39.375	39.662	31.784	1.00 21.54	С
MOTA	2447	0	ILE A 318	39.930	39.697	32.895	1.00 20.69	0
ATOM	2448	CB	ILE A 318	40.650	40.153	29.646	1.00 21.19	С
ATOM	2449		ILE A 318	41.664	39.560	28.670	1.00 21.41	С
ATOM	2450		ILE A 318	41.315	41.267	30.461	1.00 21.05	С
MOTA	2451		ILE A 318	42.217	40.569	27.663	1.00 21.73	С
ATOM	2452.	N	MET A 319	38.146		31.569	1.00 21.31	N
ATOM	2453	CA	MET A 319	37.400		32.632	1.00 21.99	C
ATOM	2454	С	MET A 319	37.094	39.787	33.748	1.00 22.21	С
ATOM	2455	0	MET A 319	37.219		34.937	1.00 23.25	. 0
ATOM	2456	CB	MET A 319	36.133		32.108	1.00 21.66	C
ATOM ATOM	2457 2458	CG SD	MET A 319	36.369		31.233	1.00 21.49	C
ATOM	2459	CE	MET A 319 MET A 319	34.787 34.192		30.787	1.00 23.05	s C
ATOM	2459	N	ARG A 320	36.736		29.453 33.379	1.00 22.63 1.00 21.99	Ŋ
ATOM	2461	CA	ARG A 320	36.492		34.383	1.00 21.57	C
ATOM	2462	C	ARG A 320	37.750		35.223	1.00 21.37	C
ATOM	2463	Ö	ARG A 320	37.669		36.439	1.00 21.22	0
ATOM	2464	СВ	ARG A 320	36.083		33.726	1.00 20.79	C
ATOM	2465	CG	ARG A 320	34.702		33.014	1.00 22.36	C
ATOM	2466	CD	ARG A 320	34.300		32.452	1.00 21.24	Ċ
MOTA	2467	NE	ARG A 320			33.558	1.00 21.37	Ŋ
ATOM	2468	CZ	ARG A 320	33.148		34.423	1.00 21.73	C
MOTA	2469	NH1	ARG A 320	32.196		34.308		N
MOTA	2470	NH2	ARG A 320	33.100	33.109	35.425	1.00 23.33	N
MOTA	2471	N	ASN A 321	38.908		34.571	1.00 21.35	N
MOTA	2472	CA	ASN A 321	40.159		35.282	1.00 21.20	. С
MOTA	2473	С	ASN A 321			36.239	1.00 21.02	С
MOTA	2474	0	ASN A 321			37.364	1.00 21.80	0
MOTA	2475	CB	ASN A 321			34.311	1.00 21.07	С
MOTA	2476	CG	ASN A 321			33.752	1.00 22.81	С
MOTA	2477		ASN A 321			34.431	1.00 23.88	0
ATOM	2478		ASN A 321			32.521	1.00 20.59	N
ATOM	2479	N	ILE A 322			35.802	1.00 20.31	И
ATOM	2480	CA	ILE A 322			36.683	1.00 19.83	C
MOTA	2481	C	ILE A 322			37.918	1.00 19.45	C
ATOM	2482 2483	0	ILE A 322 ILE A 322			39.037	1.00 18.04	0
MOTA MOTA	2483	CB CG1	ILE A 322			35.980	1.00 20.01	C
ATOM	2484		ILE A 322			34.849	1.00 21.62	C
ATOM	2485		ILE A 322			36.989 35.278	1.00 20.64 1.00 23.99	C C
ATOM	2487	И	GLU A 323	20 444		37.716	1.00 23.99	N
ATOM	2488	CA	GLU A 323			38.841		N C
ATOM	2489	C	GLU A 323					C
ATOM	2490	Ö	GLU A 323			40.980		0
ATOM	2491	СВ	GLU A 323					C
				20.050		20.200		Č

ATOM	2492	CG G	SLU A	323	3	35.478	40.987	37.787		19.24	
MOTA	2493	CD G	LU A	323	3	34.096	40.764	37.189	1.00	17.51	
ATOM			SLU A	323 -	3	33.140	40.470	37.922	1.00	17.44	
ATOM			LU A		3	33.982	40.901	35.974	1.00	16.60	
MOTA			LYS A			38.357	37.711	39.227	1.00	19.47	
			LYS A			38.781	36.570	40.037		20.33	
ATOM			LYS A			40.040	36.869	40.839		20.67	
MOTA						40.090	36.562	42.023		20.56	
ATOM			LYS A					39.172		20.11	
ATOM			LYS A			39.040	35.334			20.73	
MOTA			LYS A			37.803	34.678	38.572			
MOTA			LYS A			38.238	33.413	37.761		21.68	
MOTA			LYS A			37.117	32.866	36.857		22.30	
ATOM	2504		LYS A			37.534	31.609	36.153		19.72	
MOTA	2505		MET A			41.045	37.456	40.194		21.37	
ATOM	2506		MET A			42.305	37.782	40.860		22.78	
ATOM	2507	C	MET A	325		42.106	38.789	41.990		22.78	
MOTA	2508	0	MET A	325		42.734	38.694	43.047		22.48	
ATOM	2509	CB	MET A	325		43.308	38.369	39.865		23.14	•
MOTA	2510		MET A			43.964	37.359	38.978	1.00	27.30	
ATOM	2511		MET A			44.699	38.147	37.511	1.00	35.72	
ATOM	2512		MET A			45.804		38.338	1.00	36.16	
ATOM	2513		LEU A			41.248	39.765	41.752	1.00	23.21	
ATOM	2514		LEU A			40.977				24.47	
	2515		LEU A			40.307		43.969		24.48	
MOTA	2516		LEU A			40.659	40.500			24.21	
MOTA			LEU A			40.087		42.159		24.63	
MOTA	2517					40.618	43.282	41.988		27.80	
ATOM	2518	CG	LEU A			42.135	43.441			28.29	
ATOM	2519						43.820	40.682		28.01	
MOTA	2520		LEU A			40.038				25.29	
MOTA	2521	N	GLY A			39.350	39.314			25.73	
MOTA	2522	CA	GLY A			38.663	38.608	44.782			
MOTA	2523	С	GLY A			39.644	37.854	45.638		25.86	
ATOM	2524	0	GLY F			39.597	37.931	46.863		25.83	
MOTA	2525	N	GLU A			40.556	37.137			26.02	
ATOM	2526	CA	GLU A			41.558	36.397	45.762		26.93	
MOTA	2527	С		A 328		42.557	37.306	46.480		25.70	•
MOTA	2528	0		A 328		42.883	37.070			24.67	
ATOM	2529	CB		A 328		42.293	35.423			27.76	
ATOM	2530	CG		A 328		41.403				0 31.57	
ATOM	2531	CD	GLU A	A 328		41.635	32.992			0 37.39	
ATOM	2532	OE1	GLU Z	A 328.		42.048	33.058			0 41.34	
ATOM	2533	OE2	GLU Z	A 328	• •	41.430	31.902	44.552	1.0	0 42.69	
ATOM	2534	N		A 329		43.024	38.356	45.816	1.0	0 25.20	
ATOM	2535	CA		A 329		4.4.031	39.219	46.433	1.0	0 25.42	
ATOM	2536	С		A 329		43.475	40.039	47.582	1.0	0 25.67	
ATOM	2537	Ö		A 329		44.141			1.0	0 25.92	
ATOM	2538	СВ		A 329		44.670		45.409	1.0	0 25.31	
ATOM	2539	N		A 330		42.241			1.0	0 26.51	
ATOM	2540	CA		A 330		41.656				0 27.12	
MOTA	2541	C		A 330		41.156				0 27.74	
ATOM	2542	Ö		A 330		40.845				0 27.62	
	2542	СВ		A 330		40.517				0 27.19	
ATOM	2543	CG		A 330		40.966				0 27.69	
MOTA				A 330		39.747				0 28.15	
MOTA	2545									0 27.60	
MOTA	2546			A 330		41.774				0 28.45	
MOTA	2547	N		A 331		41.054	_			0 29.04	
ATOM	2548	CA		A 331		40.637				00 29.04	
ATOM	2549	С		A 331		39.154					
ATOM	2550	0		A 331		38.698				00 29.67	
MOTA	2551	N		A 332		38.409				00 29.16	
ATOM	2552	CA	ASN	A 332		36.973	39.190	50.243	J 1.	00 29.38	•
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TC	M	2553	С	ASN	Α	332		36.342	39.718	48.958	1.00 28.80	С
ATC		2554		ASN				36.579	40.847	48.570	1.00 28.58	ō
ATC		2555	СВ	ASN			•	36.662	40.123	51.413	1.00 29.68	Č
ATC		2556	CG	ASN				35.181	40.214	51.702	1.00 31.38	c
				ASN								
ATC		2557						34.368	39.630	50.991	1.00 35.54	0
ATC		2558				332 ·		34.820	40.944	52.751	1.00 33.23	N
ATC		2559	N	PRO				35.504	38.922	48.325	1.00 28.45	N
ATC	MC	2560	CA			333		34.944	39.288	47.025	1.00 28.38	C .
ATC	M· MC	2561	C	PRO	Α	333		34.094	40.534	47.093	1.00 28.04	С
ATC	MC	2562	0	PRO	Α	333		33.913	41.187	46.073	1.00 28.11	0
ATC	MC	2563	CB ·	PRO	Α	333		34.071	38.093	46.640	1.00 28.23	C
ATO	MC	2564	CG	PRO	Α	333		34.203	37.097	47.701	1.00 29.36	С
ATC		2565	CD			333		34.999	37.641	48.822	1.00 28.91	Ċ
ATO		2566	N			334		33.556	40.844	48.262	1.00 27.75	N
ATO		2567	CA			334		32.727	42.033	48.400	1.00 28.08	Ĉ
ATO		2568	C			334		33.582	43.282	48.300	1.00 26.62	č
ATO		2569	Õ			334		33.064	44.365	48.086	1.00 26.31	o
ATO		2570	CB			334		31.857	41.989	49.686	1.00 28.89	C
ATO		2571	CG			334		30.594	41.090	49.459	1.00 32.52	C
ATO		2572	CD			334		29.523	41.114	50.556	1.00 36.22	. C
ATO		2573	OE1			334		29.500	42.004	51.421	1.00 39.82	0
ATO		2574	NE2			334		28.612	40.127	50.503	1.00 38.24	N
ATO	MC	2575	N			335		34.894	43.138	48.414	1.00 25.23	N
ATO	MC	2576	CA	GLU	Α	335		35.763	44.290	48.269	1.00 24.55	С
ATO	MC	2577	С	GLU	Α	335		36.090	44.584	46.790	1.00 22.95	С
ATO	MC	2578	0	GLU	A	335		36.691	45.597	46.475	1.00 21.47	0
ATO	MC	2579	CB	GLU	Α	335		37.038	44.091	49.088	1.00 25.61	С
ATO		2580	CG			335		36.820	44.189	50.599	1.00 29.47	С
AT		2581	CD			335		38.115	44.280	51.369		Ċ
AT		2582				335		38.964	45.124	51.004		ŏ
AT		2583				335		38.288	43.521	52.350	1.00 40.05	ő
AT		2584	N			336		35.654	43.722	45.877	1.00 21.52	N
AT		2585	CA			336		35.993				
									43.898	44.458	1.00 20.69	C
ATO		2586	C			336		35.422	45.176	43.855	1.00 19.97	C
AT		2587	0			336		36.134	45.949	43.239	1.00 19.57	0
ATO		2588	CB			336		35.594	42.683	43.653	1.00 20.59	C
AT		2589				336		35.746	42.933	42.179	1.00 21.20	С
AT		2590				336		36.467	41.513	44.067	1.00 21.28	С
AT		2591	N			337		34.146	45.421	44.080	1.00 19.82	N
TA	MO	2592	CA			337		33.492	46.598	43.568	1.00 19.66	С
AT	MO	2593	С	GLY	Α	337		34.130	47.906	43.981	1.00 19.56	С
AT	MO	2594	0	GLY	Α	. 337		34.510	48.693	43.131	1.00 19.35	0
AT	MO	2595	N	PRO	A	338		34.202	48.162	45.278	1.00 19.93	N
AT	MO	2596	CA	PRO	Α	. 338		34.846	49.383	45.790	1.00 19.88	С
AT	OM	2597	С			. 338		36.272	49.631	45.254	1.00 19.22	С
AT		2598	0			. 338		36.591	50.758	44.908	1.00 18.43	ō
AT		2599	CB			338		34.830	49.191	47.316	1.00 19.61	Ċ
AT		2600	CG			338		33.625	48.380	47.555	1.00 20.33	Č
AT		2601	CD			. 338		33.579	47.367	46.359	1.00 20.75	c
AT		2602	N									
						. 339		37.107	48.612	45.171	1.00 19.21	N
AT		2603	CA			. 339		38.416	48.814	44.566	1.00 19.65	. C
	OM	2604	С			. 339		38.283	49.219	43.081	1.00 19.35	C
	MO	2605	0			. 339		38.927	50.188	42.621	1.00 17.91	0
. AT		2606	CB			. 339		39.279	47.570	44.693	1.00 20.38	С
	OM	2607	CG			. 339		40.745	47.814	44.291	1.00 21.96	С
AT	OM	2608	CD1	LEU	Α	. 339		41.681	47.151	45.220	1.00 25.12	С
AT	MO	2.609	CD2	LEU	Α	339		40.991	47.293	42.899	1.00 22.54	С
AT	OM	2610	N			340		37.420	48.512	42.345	1.00 19.18	N
	OM	2611	CA			340		37.231	48.821	40.928	1.00 19.26	C
	OM	2612	C			340		36.764	50.260	40.746		Č
	OM	2613	Ö			340		37.306	50.200	39.893		o
17.1	→1.3	~ O T O	9	0 نديد		. 540		57.500	50.505	29.093	1.00 10.71	J

ATOM	2614	CB LEU A 340	36.260	47.857		1.00 19.85
ATOM	2615	CG LEU A 340	36.823	46.470	39.960	1.00 21.77
ATOM	2616	CD1 LEU A 340	35.745	45.671	39.299	1.00 22.81
	2617	CD2 LEU A 340	38.088	46.539	39.072	1.00 21.14
ATOM			35.798	50.676		1.00 19.12
ATOM	2618	= -		52.052		1.00 20.43
MOTA	2619	CA ASN A·341	35.296			1.00 20.43
MOTA	2620	C ASN A 341	36.367	53.086		
ATOM	2621	O ASN A 341	36.474	54.110		1.00 19.81
MOTA	2622	CB ASN A 341	34.090	52.232		1.00 20.40
ATOM	2623	CG ASN A 341	32.814	51.659		1.00 24.06
ATOM	2624	OD1 ASN A 341	32.390	52.073	40.829	1.00 31.36
ATOM	2625	ND2 ASN A 341	32.229		42.561	1.00 25.82
ATOM	2626	N THR A 342	37.129		42.912	1.00 19.43
	2627	CA THR A 342	38.227	53.664		1.00 19.71
ATOM			39.230			1.00 19.45
MOTA	2628		39.739			1.00 19.23
MOTA	2629	O THR A 342				1.00 20.44
MOTA	2630	CB THR A 342	38.873			
MOTA	2631	OG1 THR A 342	38.030	53.322		1.00 21.13
MOTA	2632	CG2 THR A 342	40.208	53.756		1.00 20.71
MOTA	2633	N MET A 343	39.464			1.00 19.49
ATOM	2634	CA MET A 343	40.381			1.00 19.90
ATOM	2635	C MET A 343	39.932	53.649	39.164	1.00 19.94
ATOM	2636	O MET A 343	40.775	54.344	38.567	1.00 18.43
ATOM	2637	CB MET A 343	40.543	51.347	39.664	1.00 19.92
ATOM	2638	CG MET A 343	41.701	50.556	40.115	1.00 23.07
ATOM	2639	SD MET A 343	42.163	49.194	38.959	1.00 24.93
ATOM	2640	CE MET A 343	41.013	48.220	39.315	1.00 27.48
	2641	N ILE A 344	38.629	53.643	38.837	1.00 20.84
ATOM			38.159	54.412	37.679	1.00 21.51
MOTA	2642		37.624	55.800	37.918	1.00 21.46
MOTA	2643	C ILE A 344		56.639		1.00 21.65
ATOM	2644	O ILE A 344			36.805	1.00 22.58
MOTA	2645		37.089	53.641		1.00 22.50
MOTA	2646		35.714	53.723	37.435	1.00 24.03
MOTA	2647		37.506	52.220	36.555	
MOTA	2648		34.635	53.407		1.00 28.35
MOTA	2649		37.009		39.062	1.00 21.48 1.00 22.11
MOTA	2650		36.410			
MOTA	2651		37.382			1.00 20.79
ATOM	2652		38.380			1.00 20.06
MOTA	2653	CB LYS A 345	. 35.405			1.00 23.49
MOTA	2654	CG LYS A 345	35.497			1.00 28.03
MOTA	2655	CD LYS A 345	34.120		41.683	
ATOM	2656		33.282	56.986		1.00 32.44
MOTA	2657		33.859	56.977		1.00 36.32
MOTA	2658		37.062	59.501		1.00 19.28
ATOM	2659		37.911	60.636	38.013	1.00 18.60
ATOM	2660		39.222	60.254	37.350	1.00 17.41
ATOM.			40.090		37.229	1.00 18.04
ATOM	2662		39.353			1.00 17.62
MOTA	2663		40.616			1.00 17.91
	2664		40.415			1.00 18.08
MOTA			41.108			
ATOM	2665		41.284			
ATOM	2666					
MOTA	2667		41.719			
MOTA	2668		43.179			
MOTA	2669		43.165			
MOTA	2670			55.405		
MOTA	267:		45.271			
MOTA	267		43.678			
ATOM	267		39.450			
MOTA	267	4 CA TYR A 348	39.098	3 56.480	33.444	1.00 20.50

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MOTA	2675	С	TYR Z	Α	348	37.637	56.691	33.036	1.00	22.07			С
ATOM	2676	0	TYR A			37.233	56.236	31.978	1.00	22.11			0
MOTA	2677	CB	TYR A			39.311	54.963	33.478		19.77			C
MOTA	2678	CG	TYR A			40.753	54.545	33.561		20.36			С
MOTA	2679		TYR .			41.540	54.483	32.422		19.91			С
MOTA	2680		TYR .			41.335	54.225	34.780		18.20			С
ATOM	2681		TYR .			42.859	54.099	32.489		19.81			C
ATOM	2682	CE2	TYR			42.662	53.841	34.863		19.47			C
ATOM	2683	CZ	TYR .			43.425	53.785	33.711		19.43			С
MOTA	2684	OH	TYR .			44.742	53.414	33.773		15.61			0
ATOM	2685	N CA	ASN .			36.820	57.344	33.850		24.37 26.66			N C
ATOM ATOM	2686 2687	CA	ASN .			35.414 34.941	57.472 58.854	33.456 33.092		28.03			C
ATOM	2688	Ö	ASN			35.663	59.847	32.992		27.79			ō
ATOM	2689	СВ	ASN			34.498	56.919	34.518		26.23			C
ATOM	2690	CG	ASN			34.463	57.764	35.748		27.89			Č
ATOM	2691		ASN			35.247	58.718	35.927		27.38			0
ATOM	2692		ASN			33.545	57.409	36.645		32.46			N
ATOM	2693		ASN			33.736	58.963	32.900		32.44			0
TER	2694		ASN										_
MOTA	2695	'n	LEU			45.819	35.786	30.984	1.00	36.91			N
ATOM	2696	CA	LEU	S	795	44.711	36.756	31.250	1.00	37.26			С
ATOM	2697	C	LEU	S	795	43.553	36.418	30.323	1.00	37.49			С
ATOM	2698	0	LEU	S	795	42.391	36.451	30.712	1.00	36.90			0
ATOM	2699	CB	LEU	S	795	45.183	38.186	31.044	1.00	37.26			С
MOTA	2700	CG	LEU		795	44.683	39.204	32.074	1.00	37.32			С
MOTA	2701		LEU		795	44.775	38.671	33.479		37.34			С
MOTA	2702		LEU		795	45.479	40.493	32.006		37.95			С
MOTA	2703	N	THR			43.907	36.155	29.076		38.07			N
MOTA	2704	CA			796	43.029	35.548	28.076		39.17			С
MOTA	2705	С			796	42.608	34.088	28.347		38.93			С
ATOM	2706	0	THR		796	41.784	33.533	27.622		39.51		٠.	0
MOTA	2707	CB	THR			43.750	35.628	26.705		39.45			C
ATOM	2708	OG1				43.287	34.597	25.850		41.87			0
ATOM	2709		THR			45.232	35.275	26.824		40.14			C
ATOM	2710 2711	N	SER			43.154 42.770	33.451	29.369		38.98 39.24	•		N
MOTA MOTA	2711	CA C	SER SER			41.370	32.067 31.981	29.654 30.274		39.32			C
ATOM	2712	0	SER			40.901	32.905	30.274		38.28			0
ATOM	2713	СВ	SER			43.775	31.398	30.574		38.98			Ç
MOTA	2715	OG	SER			43.613		31.891		40.40			Ö
ATOM	2716	N			798	40.713	30.851	30.059		39.93			N
ATOM	2717	CA			798	39.345	30.682	30.515		40.53			C
ATOM	2718	C			798	39.088		31.183		39.72			Ċ
MOTA	2719	Ö			798	39.797		30.958		39.72			ō
MOTA	. 2720	CB			798	38.377		29.351		41.28			C
MOTA	2721	CG	TYR	S	798	38.524		28.171		44.57			C
MOTA	2722		TYR	S	798	39.574		27.261		47.13			С
ATOM	2723	CD2	TYR	S	798	37.574	28.953	27.932	1.00	47.85			С
MOTA	2724	CE1	TYR	S	798	39.692	29.219	26.163	1.00	48.81			С
MOTA	2725	CE2	TYR			37.680	28.094	26.833		50.32			C
ATOM	2726	CZ			798	38.744		25.955	1.00	49.97			С
ATOM	2727	OH			798	38.835		24.866		49.58			0
MOTA	2728	N			799	38.051		32.005		39.16			N
MOTA	2729	CA			799	37.676		32.690		38.61			С
MOTA	2730	С			799	36.588		31.868		37.26			С
ATOM	2731	0			799	36.468		30.671		36.81			0
ATOM	2732	CB			799	37.186		34.105		39.29			C
MOTA	2733	CG			799	37.303		35.048		40.55			C
ATOM	2734		ASP			36.767		34.756		41.68			0
ATOM	2735	OD2	2 ASP	S	799	37.913	27.319	36.121	1.00	45.38			0

3.0004	0726	NT.	0V0 0	0.00	35.795	26.517	32.486	1.00 3	15 61		N
MOTA	2736		CYS S								
MOTA	2737		CYS S			25.787	31.732	1.00 3			C
MOTA	2738		CYS S			25.714	32.450	1.00 3			С
MOTA	2739	0	CYS S	800	32.749	24.708	32.388	1.00 3	33.81		0
ATOM	2740	CB	CYS S	800	35.274	24.380	31.423	1.00 3	34.32		С
ATOM	2741		CYS S		35.538	23.392	32.911	1.00 3	33.88		S
MOTA	2742		GLU S			26.792	33.101	1.00 3			N
			GLU S		31.808	26.803	33.859	1.00 3			Ċ
ATOM	2743							1.00			Ċ
ATOM ·	2744		GLU S		30.551	26.980	32.991				
ATOM	2745		GLU S		30.520	27.739	32.012	1.00			0
ATOM	2746		GLU S		31.886	27.877	34.942	1.00			С
ATOM	2747	CG	GLU S	801	33.128	27.703	35.818	1.00			С
ATOM	2748	CD	GLU S	801	33.095	28.557	37.065	1.00	36.15		C
ATOM	2749	OE1	GLU S	801	32.408	28.163	38.013	1.00	35.62		0
ATOM	2750		GLU S		33.751	29.619	37.090	1.00	38.69		0
	2751	N	VAL S		29.519	26.242	33.377	1.00			N
ATOM						26.223	32.691	1.00			C
ATOM	2752	CA	VAL S		28.244						
ATOM	2753	С	VAL S		27.137	26.148	33.735	1.00		•	C
ATOM	2754	Ο.	VAL S		27.408	25.928	34.908	1.00			0
MOTA	2755	CB	VAL S	802	28.139	24.972	31.781		33.63		С
ATOM	2756	CG1	VAL S	802	29.263	24.948	30.753	1.00	32.61		C
ATOM	2757	CG2	VAL · S	802	28.165	23.682	32.624	1.00	33.77		С
ATOM	2758	N	ASN S		25.887	26.304	33.300	1.00	35.05		N
ATOM	2759	CA	ASN S		24.745	26.222	34.204		35.82		С
			ASN S		24.457	24.784	34.642		37.45		Č
ATOM	2760	C					34.387		37.12		Õ
MOTA	2761	0	ASN S		23.379	24.241					
ATOM	2762	CB	ASN S		23.490	26.836	33.573	_	35.36		C
ATOM	2763	CG	ASN S		23.548	28.344	33.506		33.54		С
MOTA	2764	OD1	ASN S	803	24.605	28.941	33.685		32.05		0
ATOM	2765	ND2	ASN S	803	22.414	28.967	33.230	1.00	29.41		N
ATOM	2766	N	ALA S	804	25.442	24.187	35.298	1.00	39.28		N
ATOM	2767	CA	ALA S		25.340	22.846	35.855	1.00	41.13		С
ATOM	2768	C		S 804	26.566	22.620	36.734		42.43		C
	2769	Ö		S 804	27.638	23.153	36.464		42.47		Ö
ATOM							34.762		41.08		č
MOTA	2770	CB	ALA :		25.277	21.791					
ATOM	2771	N		S 805	26.410		. 37.786		44.47		N
MOTA	2772	CA		S 805	27.527	21.527	38.697		45.68		C
MOTA	2773	С		S 805	28.568	20.620	38.053		46.82		С
MOTA	2774	0	PRO	S 805	28.273	19.918	37.092	1.00	47.40		0
MOTA	2775	CB	PRO	S 805	26.847	20.783	39.854	1.00	45.66		С
MOTA.	2776	CG	PRO	S 805	25.588	20.206	39.261	1.00	45.01		C
ATOM	2777	CD		S 805	25.161	21.146	38.177	1.00	44.63		с
ATOM	2778	N		S 806	29.770	20.613	38.605		48.31		N
ATOM	2779	CA		S 806	30.847	19.766	38.098		49.34		c
				S 806	30.661	18.323	38.555		49.57		Č
MOTA	2780	С									
MOTA	2781	0		S 806	29.992	18.063	39.560		50.13		0
MOTA	2782	CB.		S 806	32.215	20.311	38.574		49.85		С
MOTA	2783	CG1	ILE	S 806	32.410	20.058	40.074		50.64		С
MOTA	2784	CG2	ILE	S 806	32.327	21.816	38.250	1.00	50.45		С
ATOM	2785	CD1	ILE	S 806	33.724	20.605	40.624	1.00	51.43		С
MOTA	2786	N		S 813	29.871	8.315	36.218	1.00	46.23		N
ATOM	2787	CA		S 813	30.588	8.788	35.034		46.32		С
ATOM	2788	C		S 813	29.685	9.635			45.87		Ċ
	2789	o		S 813	28.463	9.511			45.43		o
MOTA											
MOTA	2790	CB		S 813	31.166	7.606			46.25		C
MOTA	2791	CG		S 813	32.057	6.663			46.61		C
MOTA	2792			S 813	32.444	5.423			46.51		С
ATOM	2793	CD2	LEU	S 813	33.292	7.406		1.00	45.98		С
MOTA	2794	N	GLN	S 814	30.309	10.503	33.351	1.00	45.81		N
MOTA	2795	CA		S 814	29.595	11.400		1.00	45.92		С
ATOM	2796			S 814	30.497	11.838			45.66		С
		•				•			•		

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MO1	2797	0	GLN		814	31.706	11.626	31.329		45.05		0
MOI	2798	CB	GLN	S	814	29.123	12.643	33.198		46.09		С
MOJ	2799	CG	GLN	S	814	30.265	13.531	33.696		47.32		C
MOI	2800	CD	GLN	s	814	29.781	14.722	34.520		49.22		С
MOJ	2801	OE1	GLN	S	814	29.165	14.541	35.569		50.40		0
MOI	2802	NE2	GLN	S	814 .	30.070	15.937	34.053		49.45		N
MOJ	2803	N	GLY		815	29.898	12.476	30.294		45.88		N
MOJ	2804	CA	GLY	S	815	30.621	12.956	29.135	1.00	45.84		C
MO1	2805	С	GLY	S	815	31.426	11.863	28.462		46.13		С
MO']	2806	0	GLY	S	815	30.968	10.732	28.339	1.00			0
MO1	2807	N	GLU	S	816		12.216	28.035	1.00			N
MOI	2808	CA	GLU	S	816	33.548	11.285	27.382	1.00			С
MO1	2809	С	GLU		816	33.721	9.994	28.186	1.00			С
MOI	2810	0	GLU		816	33.823	8.910	27.614		48.54		0
MOI	2811	CB	GLÜ		816	34.920	11.948	27.184		48.06		C
MOJ	2812	CG	GLU	S	816	35.783	11.312	26.102		48.93		C
MOI	2813	CD	GLU		816	37.189	11.887	26.062		49.77		С
MOJ	2814		GLU			38.031	11.413	26.848		50.86		0
MOI	2815		GLU		816	37.457	12.802	25.247		49.55		0
MO1	2816	N	GLU			33.737	10.112	29.509		49.67		N
MOI	2817	CA	GLU			33.947	8.957	30.373		50.75		C
MOI	2818	С	GLU			32.786	7.982	30.309		51.10		C
MO3	2819	0			817	32.989	6.771	30.278		51.12		0
MOJ	2820	CB	GLU			34.164	9.406	31.815		50.97		C
MOI	2821	CG			817	35.476	10.140			52.22		C
MOJ	2822	CD	GLU			35.395	11.637	31.764		54.47		C
MOJ	2823	OE1				34.289	12.166	31.489		55.57		0
MOJ	2824		GLU			36.456	12.296	31.833		56.41	_	0
MOJ	2825	N			818	31.572	8.521	30.295		51.81		И С
MO7	2826	CA			818	30.376	7.706	30.204		52.37 53.14		C
MOI	2827	C	LEU			30.399	6.929 5.714	28.901 28.894		53.14		0
MOI MOI	2828 2829	O CB	LEU LEU			30.216 29.116	8.575	30.258		52.25		c
COM	2830	CG			818	27.786	7.814	30.236		52.23		C
MO?	2831	CD1			. 818	27.7661	6.836	31.335		52.37		c
MOE	2832	CD2			818	26.596	8.749	30.173		51.16		č
MO	2833	N	LEU			30.660	7.643	27.809	1.00			N
MOS	2834	CA			819	30.623	7.068	26.465		54.73		Ċ
OM:	2835	C	LEU			31.573	5.874	26.295		55.32		Ċ
OM	2836	Ö	LEU			31.171	4.823	25.794		55:08		ō
OM.	2837	СВ	LEU			30.929	8.162	25.426		54.66		Ċ
OM.	2838	CG			819	30.838	7.789	23.942	1.00	54.90		С
MO!	2839				819	29.480	7.239	23.559		54.56		С
MO:	2840				819	31.170	8.997	23.088	1.00	55.68		С
MO!	2841	N	ARG	S	820	32.821	6.036	26.725	1.00	55.92		N
MO:	2842	CA	ARG	; S	820	33.817	4.987	26.576	1.00	56.75		С
MO:	2843	C	ARG	; 5	820	33.488	3.762	27.428	1.00	56.92		С
MO:	2844	0	ARG	; S	820	33.578	2.617	26.951	1.00	56.86		0
MO:	2845	CB	ARG	; S	820	35.207	5.530	26.915	1.00	57.13		С
MO:	2846	CG			820	35.638	6.596	25.927	1.00	58.55		C
MO!	2847	CD			820	37.073		26.036		60.19		С
MO:	2848	NE			820	37.336				62.23		N
MO:	2849	CZ			820	38.465		25.039		64.08		С
MO.	2850				820	39.475				64.81		N
MO:	2851				820	38.586				64.58		N
MO:	2852	N			821	33.109				56.90		N
MO:	2853	CA			821	32.713				56.79		С
MO:	2854	С			821	31.611				56.74		C
MO:	2855	0			821	31.665				56.66		0
MO:	2856	CB			821	32.236				56.66		C
MO:	2857	N	LEU	JS	s 822	30.629	2.806	28.317	1.0	0 56.51		N

						_		_	155	07.	.0.7	1 00	E 6	E 0		C
	· -	2858	CA	LEU S			29.537		.155	27.6		1.00				C C
		2859	С	LEU S			30.031		.473	26.3 25.9		1.00				0
		2860	0	LEU S			29.482		.451	27.2		1.00				C
		2861	CB	LEU :			28.451 27.681		.167 .779	28.4		1.00				c
•		2862	CG CD1	LEU					.612	27.8		1.00				Č
		2863		LEU :			26.543 27.156	•	2.717	29.3		1.00				Ċ
		2864	CDZ	LEU			27.130	, 2	/ . /	23	,,,	1.00	55	.00		_
	TER HETATM	2865	E E	FE2			23.313	27	671	.28.	779	1.00	22	.12		FE
	HETATM		C1	AKG			22.355		3.315	27.		1.00				C
	HETATM		01	AKG			23.449		3.880	27.		1.00				0
	HETATM		02	AKG			22.172		1.103	2.7 .		1.00				0
	HETATM		C2	AKG			21.128		5.999	28.		1.00				С
	HETATM		05	AKG			21.211		7.117	28.		1.00				0
	HETATM		C3	AKG			19.829		5.231	28.		1.00	23	.46		С
	HETATM		C4	AKG			18.717		5.967	29.		1.00	22	.15		С
	HETATM		C5	AKG	A13	51	17.35	1 -2	5.435	28.	649	1.00	23	.90		С
	HETATM		03	AKG			17.13	6 2	4.674	27.	706	1.00	23	.27		0
	HETATM		04	AKG	A13	51	16.35	3 2	5.844		406	1.00				0
	HETATM		s	SO4	A13	52	0.19		5.255	43.	681	1.00				S
	HETATM	2878	01	SO4	A13	52	1.04		6.078		531	1.00				0
	HETATM	2879	02	SO4	A13	52	1.02		4.391		840	1.00				0
	HETATM	2880	03	SO4	A13	52	-0.64		4.431		542	1.00			•	0
	HETATM	2881	04	SO4			-0.63		6.114		830	1.00	_			0
	HETATM		S	SO4			1.93		8.607		759	1.00				S
	HETATM		01		A13		3.16		9.179		298	1.00				. 0
	HETATM		02	SO4			2.22		7.552		793	1.00				0
	HETATM		03		A13		1.18		8.079		902	1.00				0
	HETATM		04		A13		1.14		9.630		081	1.00		1.49		0
	HETATM		0	нон		1	38.42		3.864 5.366		899 554			4.59		0
	HETATM		0	НОН		2	38.02 34.91		0.689		190			4.36		ŏ
	HETATM			НОН НОН		3 4	20.48		7.037		306			5.20		ŏ
	HETATM HETATM			HOH		5	21.06		4.447		916			3.55		Ö.
	HETATM			НОН		6	29.97		4.394		.721			3.81		0
	HETATM			нон		7	29.34		8.985		744			6.25		0
	HETATM			НОН		8	35.53		3.904		.157			2.65		0
	HETATM			нон		9	33.80		-1.383		.877			5.05		0
	HETATM			НОН		1	11.56		21.626		.846	1.0	0 4	1.47	•	0
	HETATM			нон		2	9.59		21.877	12	.314	1.0	o 6	1.59		0
	HETATM			нон		3	1.32		21.339	7	. 657	1.0	0 5	8.53		0
	HETATN			нон		4	3.57		13.365		.778			7.77		0
	HETATN			НОН	Z	5	4.5		16.855		.766			1.50		0
	HETATN	1 2901	. 0	HOH	Z	6	2.40		19.552		.161			6.40		0
	HETATI			HOH		7	1.2		29.413		.184			2.18		0
	HETATI			HOH		8	2.0		32.304		.875			1.43		0
	HETATI	1 2904	1 0	HOH		9	11.5		44.907		.867			7.18		0
	HETAT			HOF		10	11.6		3.238		.221			3.99		0
	HETATI			HOF		11	3.7		32.951		.375			2.66		0
	HETAT				ı Z	12	4.8		37.611		.421			3.47		0
	HETATI				ΗZ	13	11.0		35.734		.393			34.95		0
	HETATI				H Z	14	15.5		46.392		.481			13.01		0
	HETAT				HZ	15	12.2		41.979		.720 .661			33.94 18.46		0
	HETAT				H Z	16	13.8		4.815		.755			14.45		0
	HETAT				HZ	17	15.8 13.4		22.030		.390			59.18		Ö
	HETAT				HZ	18 10	14.7		26.33		.845			51.42		ŏ
	HETAT			· HO	HZ	19 20	17.0		29.99		603			54.07		ŏ
	HETAT				n Z	21	21.1		23.98		.773			46.32		ŏ
	HETAT HETAT				n Z	22	27.5		31.13		.026			64.13		ŏ
	HETAT				HZ.	23	27.3		22.24		3.414			79.43		Ō
	ne lat	rı 231	5 0	AU.	4	ں ے	27.5				3		_			-

HETATM	2919	0	HOH Z	24	36.742	29.331	21.279	1.00 50.70	0
HETATM	2920	0	HOH Z	25	30.029	33.533	9.206	1.00 50.33	0
HETATM		0	HOH Z	26	29.955	37.104	10.551	1.00 70.40	0
HETATM		0	HOH Z	27	18.215	15.129	13.036	$1.00 \cdot 37.33$	0
HETATM		0	нон z	28	29.069	5.533	17.355	1.00 44.84	0
HETATM		0	HOH Z	29	18.941	14.771	16.383	1.00 31.41	0
HETATM		0	HOH Z	30	13.624	7.655	18.343	1.00 46.45	0
HETATM		0	HOH Z	31	5.649	12.667	27.758	1.00 44.15	0
HETATM		0	HOH Z	32	18.818	6.772	36.717	1.00 51.59	0
HETATM		0	HOH Z	33	7.620	14.589	19.463	1.00 50.93	0
HETATM		0	HOH Z	34	20.087	9.746	36.974	1.00 52.81	0
HETATM		0	HOH Z	35	21.912	13.173	44.511	1.00 59.64	0
HETATM		0	HOH Z	36	29.233	39.992	16.108	1.00 75.75	0
HETATM HETATM		0	HOH Z	37 38	33.785 15.613	44.067 37.779	25.671 35.493	1.00 62.06	0
HETATM		0	HOH Z	39	8.070			1.00 52.50	. 0
HETATM		0	HOH Z	40	16.339	38.292 30.957	35.056 40.378	1.00 60.61 1.00 43.15	0
HETATM		0	HOH Z	41	28.116	27.147	37.617	1.00 43.15	0
HETATM		0	HOH Z	42	29.707	30.087	39.279	1.00 54.89	0
HETATM		0	HOH Z	43	28.116	24.509	42.048	1.00 54.89	0
HETATM		0	HOH Z	44	25.074	24.801	42.258	1.00 53.13	0
HETATM		Ö	HOH Z	45	33.873	31.493	39.077	1.00 34.81	0
HETATM		0	HOH Z	46	31.533	33.860	46.118	1.00 43.97	0
HETATM		0	HOH Z	47	13.319	35.957	31.390	1.00 30.03	0
HETATM		Ö	HOH Z	48	27.155	38.119	52.311	1.00 44.72	0
HETATM		Ö	HOH Z	49	24.587	38.767	49.612	1.00 50.58	0
HETATM		Ö	HOH Z	50	21.687	17.630	48.071	1.00 30.36	0
HETATM		Ö	HOH Z	51	21.437	14.872	40.880	1.00 60.20	Ö
HETATM		ŏ	HOH Z	52	24.790	15.406	39.359	1.00 78.81	Ö
HETATM		Ö	HOH Z	53	23.347	17.356	36.625	1.00 52.48	. 0
HETATM		ō	HOH Z	54	21.628	10.475	34.469	1.00 47.30	Ō
HETATM		ō	HOH Z	55	18.013	-1.527	33.036	1.00 61.93	Ö
HETATM		ō	HOH Z	56	16.101	-0.104	30.078	1.00 59.33	Ö
HETATM		ŏ	HOH Z	57	26.268	5.539	16.988	1.00 38.42	Ō
HETATM		ŏ	HOH Z	58	30.916	16.527	11.437	1.00 44.01	Ō
HETATM		ō	HOH Z	59	32.683	13.953	20.664	1.00 50.04	Ō
HETATM		ō	HOH Z	60	36.797	10.766	7.771	1.00 80.75	0
HETATM		0	HOH Z	61	33.878	26.222	17.133	1.00 45.23	Ō
HETATM		0	HOH Z	62	13.442	21.089	28.459	1.00 36.04	0
HETATM		0	HOH Z	63	3.999	21.370	30.471	1.00 47.33	0
HETATM	2959	0	HOH Z	64	30.697	38.141	33.290	1.00 31.70	0
HETATM	2960	0	HOH Z	65	26.005	26.456	26.227	1.00 28.76	0
HETATM	2961	0	HOH Z	66	36.729	32.146	33.280	1.00 42.61	0
HETATM	2962	0	HOH Z	67	35.846	25.574	27.896	1.00 34.95	0
HETATM	2963	0	HOH Z	68	36.793	26.712	21.173	1.00 33.97	0
HETATM	2964	0	HOH Z	69	. 17.427	17.022	18.148	1.00 31.28	0
HETATM	2965	0	HOH Z	70	9.904	13.694	19.533	1.00 41.70	0
HETATM	2966	0	HOH Z	71	5.361	16.931	22.051	1.00 43.04	0
HETATM	2967	0	HOH Z	72	7.094	16.984	20.250	1.00 43.57	0
HETATM	2968	0	HOH Z	73	6.562	22.961	22.902	1.00 42.74	0
HETATM		0	HOH Z	74	29.508	38.942	26.471	1.00 26.72	0
HETATM		0	HOH Z		30.732	39.209	19.135	1.00 37.64	0
HETATM		0	HOH Z		26.368	42.318	17.836	1.00 57.14	0
HETATM		0	HOH Z		27.688	44.616	31.257	1.00 30.61	0
HETATM		0	HOH Z		30.230	44.988	25.170	1.00 39.14	0
HETATM		0	HOH Z		27.780	48.720	30.030	1.00 38.89	0
HETATM		0	нон z		25.931	50.741	30.611	1.00 40.27	0
HETATM		0	HOH Z		18.521	38.529	36.775	1.00 43.87	0
HETATM		0	HOH Z		26.678	31.402	38.482	1.00 36.08	0
HETATM		0	HOH Z		30.586	30.409	36.592	1.00 32.57	0
HETATM	2979	0	HOH Z	84	29.411	37.141	35.473	1.00 26.16	0

HETATM 2980 O	нон Z 85	19.821	31.713	33.874	1.00 34.80
HETATM 2981 O				33.379	1.00 32.92
		21.063	42.853	40.110	1.00 41.23
		17.544	37.859	32.276	1.00 35.87
HETATM 2983 O	·	9.230	41.082	35.833	1.00 51.41
HETATM 2984 O			43.744	27.890	1.00 70.60
HETATM 2985 C		9.313			1.00 40.87
HETATM 2986 C		12.728	42.598	26.938	
HETATM 2987 C		15.113	37.993	32.591	1.00 35.55
HETATM 2988 C	о нон z 93	10.676	48.283	31.613	1.00 62.24
HETATM 2989 C	о нон z 94	15.611	44.853	34.883	1.00 32.72
HETATM 2990 C	о нон z 95	15.874	51.836	39.217	1.00 66.58
	о нон z 96	15.796	47.224	39.264	1.00 52.95
	о нон z 97	26.624	53.557	28.816	1.00 69.05
	о нон z 98	15.381	50.418	22.170	1.00 36.68
	о нон z 99	15.121	55.730	27.489	1.00 51.35
	O HOH Z 100	18.542	56.170	28.175	1.00 58.02
	о нон z 101	23.731	46.355	19.907	1.00 39.06
	O HOH Z 102	16.618	46.781	22.039	1.00 33.91
		26.585	40.624	15.634	1.00 69.17
		12.758	29.333	13.489	1.00 35.42
		10.886	19.245	14.132	1.00 51.89
••••	O HOH Z 105			13.245	1.00 33.88
	о нон z 106	19.776	18.049	12.190	1.00 40.50
	о нон z 107	14.725	18.642		1.00 40.30
	O HOH Z 108	27.783	27.681	24.556	1.00 27.24
	O HOH Z 109	35.999	32.896	30.270	
HETATM 3005	O HOH Z 110	30.237	36.282	26.881	1.00 28.77
HETATM 3006	O HOH Z 111	32.759	34.258	19.346	1.00 47.40
HETATM 3007	O HOH Z 112	27.418	30.315	25.756	1.00 27.70
HETATM 3008	O HOH Z 113	16.248	36.360	29.657	
HETATM 3009	O HOH Z 114	7.438	31.072	24.792	1.00 43.13
HETATM 3010	O HOH Z 115	7.743	30.565	27.379	
HETATM 3011	O HOH Z 116	5.158	19.080	24.012	1.00 45.77
HETATM 3012	O HOH Z 117	6.366	24.013	25.459	1.00 41.84
HETATM 3013	O HOH Z 118	42.594	37.813	18.527	
HETATM 3014	O HOH Z 119	42.361		19.742	1.00 59.24
HETATM 3015	O HOH Z 120	34.674			1.00 53.99
	O HOH Z 121	33.762			1.00 39.85
HETATM 3016			39.446		
HETATM 3017	•	37.674			
HETATM 3018		38.677			and the second s
HETATM 3019		41.375			
HETATM 3020	O HOH Z 125		40.559		
HETATM 3021				42.134	
HETATM 3022					
HETATM 3023		41.949	60.812		
HETATM 3024			53.394	32.063	
HETATM 3025		37.841	55.408	29.621	1.00 45.14
CONECT 1482			•		
CONECT 1502	2866		•		
CONECT 2171	2866				
CONECT 2866	2871 2868 1482	2171 1502			
CONECT 2867	2868 2869 2870		•		
CONECT 2868	2867 2866				
CONECT 2869					
CONECT 2870	2867 2871 2872				
CONECT 2871				-	
CONECT 2872	2870 2873				
CONECT 2873	2872 2874				
CONECT 2874	2873 2875 2876				
CONECT 2875	2874				
CONECT 2876					
CONECT 2070	2878 2879 2880	2881			
CONECT 2011	2010 2015 2000	2004			

CONECT	2878	2877										•
CONECT	2879	2877										
CONECT	2880	2877										
CONECT	2881	2877										
CONECT	2882	2883	2884	2885	2886							
CONECT	2883	2882		•								
CONECT	2884	2882										
CONECT	2885	2882										
CONECT	2886	2882										
MASTER		437	0	4	15	20	0	7	6 3023	2	24	31
END												•

Structure 3

Below are the coordinates for structure 3 (the 2.5 Å structure of FIH: Zn(II): NOG: CAD):

```
12-AUG-02
                                                              1H2M
          TRANSCRIPTION ACTIVATOR/INHIBITOR
HEADER
         FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX WITH HIF-1 ALPHA
TITLE
         2 FRAGMENT PEPTIDE
TITLE
COMPND
         MOL ID: 1;
         2 MOLECULE: FACTOR INHIBITING HIF1;
COMPND
         3 SYNONYM: FIH1;
COMPND
         4 CHAIN: A;
COMPND
         5 ENGINEERED: YES;
COMPND
COMPND
         6 MOL ID: 2;
         7 MOLECULE: HYPOXIA-INDUCIBLE FACTOR 1 ALPHA;
COMPND
        8 SYNONYM: HIF-1 ALPHA, ARNT INTERACTING PROTEIN,
COMPND
        9 MEMBER OF PAS PROTEIN 1, MOP1, HIF1 ALPHA, HIF1A.
COMPND
COMPND 10 CHAIN: S;
COMPND 11 FRAGMENT: C-TERMINAL TRANSACTIVATION DOMAIN FRAGMENT
COMPND 12 RESIDUES 775 - 826
SOURCE
         MOL ID: 1;
         2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE
        3 ORGANISM_COMMON: HUMAN;
SOURCE
         4 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE
        5 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE
         6 EXPRESSION_SYSTEM_PLASMID: PET28A(+);
SOURCE
SOURCE
         7 MOL ID: 2;
         8 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
 SOURCE
        9 ORGANISM COMMON: HUMAN;
 SOURCE
 SOURCE 10 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
 SOURCE 11 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
 SOURCE 12 EXPRESSION SYSTEM PLASMID: PGEX-GP-1
           FIH, HIF, DSBH, OXYGENASE, TRANSCRIPTION, HYPOXIA,
 KEYWDS
          2 2-OXOGLUTARATE, ASPARAGINYL HYDROXYLASE, HYDROXYLASE
 KEYWDS
           X-RAY DIFFRACTION
 EXPDTA
           J.M.ELKINS, K.S.HEWITSON, L.A.MCNEILL, I.SCHLEMMINGER,
 AUTHOR
          2 J.F.SEIBEL, C.J.SCHOFIELD
 AUTHOR
              04-SEP-02 1H2M
 REVDAT
                               0
                    J.M.ELKINS, K.S.HEWITSON, L.A.MCNEILL,
 JRNL
             AUTH 2 I.SCHLEMMINGER, J.F. SEIBEL, C.J. SCHOFIELD
 JRNL
             TITL FIH: HIF-FRAGMENT COMPLEXES
 JRNL
                    TO BE PUBLISHED
             REF
 JRNL
             REFN
 JRNL
 REMARK
          2 RESOLUTION. 2.5 ANGSTROMS.
 REMARK
 REMARK
          3 REFINEMENT.
 REMARK
                           : REFMAC 5.0
          3
              PROGRAM
 REMARK
                           : MURSHUDOV, VAGIN, DODSON
              AUTHORS
           3
 REMARK
           3
 REMARK
                REFINEMENT TARGET : MAXIMUM LIKELIHOOD
  REMARK
           3
  REMARK
           3
              DATA USED IN REFINEMENT.
           3
  REMARK
               RESOLUTION RANGE HIGH (ANGSTROMS) :
                                                     2.50
  REMARK
               RESOLUTION RANGE LOW (ANGSTROMS): 18.00
           3
  REMARK
                                       (SIGMA(F)) : NONE
           3
               DATA CUTOFF
  REMARK
               COMPLETENESS FOR RANGE
                                             (%): 99.68
  REMARK
           3
                                                    18404
               NUMBER OF REFLECTIONS
           3
  REMARK
  REMARK
           3 FIT TO DATA USED IN REFINEMENT.
  REMARK
```

```
CROSS-VALIDATION METHOD
                                              : THROUGHOUT
 MARK
       3
EMARK
          FREE R VALUE TEST SET SELECTION : RANDOM
       3
          R VALUE (WORKING + TEST SET) : 0.19432
EMARK
        3
EMARK
          R VALUE
                        (WORKING SET) : 0.19185
        3
                                              : 0.22491
EMARK
        3
          FREE R VALUE
          FREE R VALUE TEST SET SIZE
                                         (%) : 7.6
EMARK
          FREE R VALUE TEST SET COUNT : 1516
EMARK
        3 FIT IN THE HIGHEST RESOLUTION BIN.
EMARK
          TOTAL NUMBER OF BINS USED
                                                       20
EMARK
                                                     2.500
.EMARK
            BIN RESOLUTION RANGE HIGH
         BIN RESOLUTION RANGE LOW
EMARK
        3 REFLECTION IN BIN (WORKING SET) :
EMARK
                                  (WORKING SET) :
        3 BIN R VALUE
EMARK
           BIN FREE R VALUE SET COUNT
                                                 :
.EMARK
        3 BIN FREE R VALUE
                                                     0.297
EMARK
.EMARK
        3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
.EMARK
                       : 2979
.EMARK
        3
          ALL ATOMS
.EMARK
        3
        3 B VALUES.
EMARK
           FROM WILSON PLOT (A**2): NULL MEAN B VALUE (OVERALL, A**2): 35.778
                                       (A**2) : NULL
EMARK
EMARK
:EMARK
           OVERALL ANISOTROPIC B VALUE.
EMARK
            B11 (A^{**}2) : -0.68
             B22 (A**2):
EMARK
                             -0.68
                             1.35
EMARK
        3
             B33 (A**2) :
EMARK
             B12 (A**2) :
        3
                              0.00
             B13 (A**2) :
EMARK
        3
EMARK
        3
             B23 (A**2) :
EMARK
        3
EMARK
        3 ESTIMATED OVERALL COORDINATE ERROR.
        3 ESU BASED ON R VALUE
LEMARK
                                                              (A): 0.334
EMARK
                                                              (A): 0.233
           ESU BASED ON FREE R VALUE
        3
REMARK
                                                                     0.224
        3
            ESU BASED ON MAXIMUM LIKELIHOOD
                                                              (A):
            ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2): 9.825
REMARK
       3
EMARK 3
REMARK 3 CORRELATION COEFFICIENTS.
REMARK 3 CORRELATION COEFFICIENT FO-FC : 0.948
REMARK 3
            CORRELATION COEFFICIENT FO-FC FREE: 0.935
≀EMARK 3
                                                 COUNT RMS
LEMARK
                                                                    WEIGHT
        3 RMS DEVIATIONS FROM IDEAL VALUES
                                               (A): 2957; 0.017; 0.021
REMARK 3 BOND LENGTHS REFINED ATOMS
                                               (A): 2546; 0.001; 0.020
REMARK 3 BOND LENGTHS OTHERS
REMARK 3 BOND ANGLES REFINED ATOMS (DEGREES): 4022; 1.612; 1.948
            BOND ANGLES OTHERS (DEGREES): 5944; 0.832; 3.000
LEMARK
            TORSION ANGLES, PERIOD 1 (DEGREES): 350; 4.024; 3.000 TORSION ANGLES, PERIOD 3 (DEGREES): 512;18.015;15.000 CHIRAL-CENTER RESTRAINTS (A**3): 413; 0.097; 0.200
LEMARK
EMARK
LEMARK
            GENERAL PLANES REFINED ATOMS
GENERAL PLANES OTHERS
                                                (A): 3315; 0.006; 0.020
EMARK
                                                      602 ; 0.002 ; 0.020
≀EMARK
                                                (A):
                                                      731 ; 0.232 ; 0.300
≀EMARK
             NON-BONDED CONTACTS REFINED ATOMS (A):
             NON-BONDED CONTACTS OTHERS
                                                (A): 2492; 0.214; 0.300
₹EMARK
         3
                                                (A): 193; 0.173; 0.500

(A): 6; 0.126; 0.500

(A): 2; 0.054; 0.500

(A): 15; 0.194; 0.300

(A): 54; 0.255; 0.300
≀EMARK
         3
             H-BOND (X...Y) REFINED ATOMS
             H-BOND (X...Y) OTHERS
≀EMARK
         3
             POTENTIAL METAL-ION REFINED ATOMS (A):
₹EMARK
             SYMMETRY VDW REFINED ATOMS (A):
SYMMETRY VDW OTHERS (A):
LEMARK
         3
≀EMARK
             SYMMETRY H-BOND REFINED ATOMS (A): 7; 0.244; 0.500
SYMMETRY H-BOND OTHERS (A): 1; 0.053; 0.500
≀EMARK
LEMARK
         3
₹EMARK
         3
```

```
3 ISOTROPIC THERMAL FACTOR RESTRAINTS. . COUNT RMS
                                                               WEIGHT
REMARK
          MAIN-CHAIN BOND REFINED ATOMS (A**2): 1767; 0.761; 1.500
REMARK
        3 MAIN-CHAIN ANGLE REFINED ATOMS (A**2): 2846; 1.421; 2.000
REMARK
           SIDE-CHAIN BOND REFINED ATOMS (A**2): 1190; 2.220; 3.000
REMARK
           SIDE-CHAIN ANGLE REFINED ATOMS (A**2): 1176; 3.678; 4.500
REMARK
REMARK
        3 NCS RESTRAINTS STATISTICS
REMARK
           NUMBER OF NCS GROUPS : NULL
REMARK
REMARK
        3
REMARK
          TLS DETAILS
        3
           NUMBER OF TLS GROUPS : 1
REMARK 3
REMARK 3
           TLS GROUP :
REMARK 3
           NUMBER OF COMPONENTS GROUP :
REMARK 3
                        C SSSEQI TO C SSSEQI
           COMPONENTS
REMARK 3
           RESIDUE RANGE:
                                           A 451
                            Α
                                 15
REMARK 3
           RESIDUE RANGE : S
                                            S
                                                822
                                 795
REMARK 3
REMARK 3 ORIGIN FOR THE GROUP (A): 22.5990 26.9200 28.6340
            T TENSOR
       3
REMARK
                                 0.0302
            T11: 0.1903 T22:
        3
REMARK
             T33: 0.0452 T12: -0.0025
T13: -0.0536 T23: 0.0309
        3
REMARK
        3 T13: -
3 L TENSOR
        3
REMARK
REMARK
            L11: 0.7638 L22: 2.2674
REMARK
        3
             L33: 1.0629 L12: 0.7977
REMARK
        3
                     0.4200 L23: 1.0769
        3
              L13:
REMARK
         3 S TENSOR
REMARK
             S11: 0.0306 S12: -0.1225 S13: -0.0490
REMARK
               S21: 0.1656 S22: 0.0303 S23: 0.0478
         3
REMARK
               S31: 0.2046 S32: 0.0231 S33: -0.0609
REMARK
         3
 REMARK
         3 BULK SOLVENT MODELLING.
 REMARK
         3 METHOD USED : BABINET MODEL WITH MASK
 REMARK
         3 PARAMETERS FOR MASK CALCULATION
 REMARK
 REMARK 3 VDW PROBE RADIUS : 1.40
 REMARK 3 ION PROBE RADIUS : 0.80
 REMARK 3 SHRINKAGE RADIUS
                                  0.80
       3
 REMARK
         3 OTHER REFINEMENT REMARKS:
 REMARK
         3 HYDROGENS HAVE BEEN ADDED IN THE RIDING POSITIONS
 REMARK
 REMARK
        4 1H2M COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
 REMARK
 REMARK 100
 REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY EBI ON 12-AUG-2002.
 REMARK 100 THE EBI ID CODE IS EBI-11173.
 REMARK 200
 REMARK 200 EXPERIMENTAL DETAILS
                                        : X-RAY DIFFRACTION
 REMARK 200 EXPERIMENT TYPE
           DATE OF DATA COLLECTION : 15-MAY-2002
 REMARK 200
                                 (KELVIN) : 100
 REMARK 200 TEMPERATURE
 REMARK 200 PH
                                         : 7.5
 REMARK 200 NUMBER OF CRYSTALS USED
                                     · : 1
 REMARK 200
                                    (Y/N) : Y
 REMARK 200 SYNCHROTRON
                                          : SRS BEAMLINE PX9.6
 REMARK 200 RADIATION SOURCE
                                          : PX9.6
 REMARK 200 BEAMLINE
                                         : NULL
 REMARK 200 X-RAY GENERATOR MODEL
                                  (M/L) : M
 REMARK 200 MONOCHROMATIC OR LAUE
 REMARK 200 WAVELENGTH OR RANGE
                                     (A) : 0.87
                                          : NULL
  REMARK 200 MONOCHROMATOR
  REMARK 200 OPTICS
                                          : NULL
```

```
REMARK 200
                                         : ADSC QUANTUM 4
           DETECTOR TYPE
REMARK 200
REMARK 200 DETECTOR MANUFACTURER
                                           : ADSC
REMARK 200 INTENSITY-INTEGRATION SOFTWARE: MOSFLM
REMARK 200 DATA SCALING SOFTWARE
                                           : SCALA
REMARK 200
                                          : 20058
REMARK 200 NUMBER OF UNIQUE REFLECTIONS
REMARK 200 RESOLUTION RANGE HIGH
                                       (A) : 2.50
                                        (A): 87.71
REMARK 200 RESOLUTION RANGE LOW
REMARK 200 REJECTION CRITERIA (SIGMA(I)) : NONE
REMARK 200
REMARK 200 OVERALL.
                                        (%) : 99.7
REMARK 200
           COMPLETENESS FOR RANGE
REMARK 200
           DATA REDUNDANCY
                                            : 6.5
REMARK 200
                                        (I) : 0.050
           R MERGE
REMARK 200
           R SYM
                                        (I) : NULL
REMARK 200
            <I/SIGMA(I) > FOR THE DATA SET : 10.7
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A): 2.50
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A): 2.64
REMARK 200
            COMPLETENESS FOR SHELL
                                        (%): 97.9
REMARK 200
            DATA REDUNDANCY IN SHELL
                                            : 4.4
REMARK 200
            R MERGE FOR SHELL
                                        (I): 0.289
REMARK 200
            R SYM FOR SHELL
                                        (I) : NULL
                                            : 2.6
REMARK 200
            <I/SIGMA(I)> FOR SHELL
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR REPLACEMENT
REMARK 200 SOFTWARE USED: NULL
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS (%): 63
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 3.4
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: 1.2M AMMONIUM SULPHATE,
REMARK 280 4% PEG400, 0.1M HEPES PH7.5, 11MG/ML PROTEIN WITH
REMARK 280
           1MM FE(II), 2.5MM NOG AND 2.5MM PEPTIDE
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 41 21 2
REMARK 290
REMARK 290
                 SYMOP
                         SYMMETRY
                         OPERATOR
 REMARK 290
                MMMMNN
 REMARK 290
                  1555
                         X, Y, Z
 REMARK 290
                  2555
                         -X, -Y, 1/2+Z
 REMARK 290
                  3555
                         1/2-Y, 1/2+X, 1/4+Z
 REMARK 290
                  4555
                         1/2+Y, 1/2-X, 3/4+Z
 REMARK 290
                  5555
                        1/2-X,1/2+Y,1/4-Z
 REMARK 290
                  6555
                         1/2+X, 1/2-Y, 3/4-Z
 REMARK 290
                  7555
                         Y, X, -Z
 REMARK 290
                  8555
                         -Y, -X, 1/2-Z
 REMARK 290
 REMARK 290
                WHERE NNN -> OPERATOR NUMBER
 REMARK 290
                      MMM -> TRANSLATION VECTOR
 REMARK 290
 REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
 REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
```

```
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
                         1 1.000000 0.000000 0.000000
                                                                             0.00000
REMARK 290
               SMTRY1
                                                                            0.00000
               SMTRY2 1 0.000000 1.000000 0.000000
REMARK 290
                                                                            0.00000
REMARK 290 SMTRY3 1 0.000000 0.000000 1.000000
REMARK 290 SMTRY1 2 -1.000000 0.000000 0.000000
                                                                            0.00000
REMARK 290 SMTRY2 2 0.000000 -1.000000 0.000000
                                                                            0.00000
REMARK 290 SMTRY3 2 0.000000 0.000000 1.000000 REMARK 290 SMTRY2 3 1.000000 0.000000 0.000000 REMARK 290 SMTRY3 3 0.000000 0.000000 1.000000 REMARK 290 SMTRY3 3 0.000000 0.000000 1.000000 REMARK 290 SMTRY1 4 0.000000 1.000000 0.000000 REMARK 290 SMTRY2 4 -1.000000 0.000000 0.000000
                                                                            74.13000
                                                                           43.12450
                                                                           43.12450
                                                                           37.06500
                                                                           43.12450
                SMTRY2 4 -1.000000 0.000000 0.000000
SMTRY3 4 0.000000 0.000000 1.000000
SMTRY1 5 -1.000000 0.000000 0.000000
                                                                           43.12450
                                                                         111.19500
REMARK 290
                                                                          43.12450
REMARK 290
                SMTRY2 5 0.000000 1.000000 0.000000
                                                                            43.12450
REMARK 290
                SMTRY3 5 0.000000 0.000000 -1.000000
SMTRY1 6 1.000000 0.000000 0.000000
                                                                            37.06500
REMARK 290
                                                                            43.12450
REMARK 290
                SMTRY2 6 0.000000 -1.000000 0.000000
                                                                          43.12450
REMARK 290
                SMTRY3 6 0.000000 0.000000 -1.000000 ...111.19500
REMARK 290
                SMTRY1 7 0.000000 1.000000 0.000000
                                                                             0.00000
 REMARK 290

      SMTRY1
      7
      0.000000
      1.000000
      0.000000

      SMTRY2
      7
      1.000000
      0.000000
      -1.000000

      SMTRY3
      7
      0.000000
      -1.000000
      -1.000000

      SMTRY1
      8
      0.000000
      -1.000000
      0.000000

      SMTRY2
      8
      -1.000000
      0.000000
      -1.000000

      SMTRY3
      8
      0.000000
      0.000000
      -1.000000

                                                                             0.00000
 REMARK 290
                                                                             0.00000
 REMARK 290
                                                                            0.00000
 REMARK 290
                                                                            0.00000
 REMARK 290
                                                                           74.13000
 REMARK 290
 REMARK 290
 REMARK 290 REMARK: NULL
 REMARK 300
 REMARK 300 BIOMOLECULE: 1
 REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
 REMARK 300 WHICH CONSISTS OF 2 CHAIN(S). SEE REMARK 350 FOR
 REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
 REMARK 300
 REMARK 300 QUATERNARY STRUCTURE FOR THIS ENTRY: TETRAMERIC
 REMARK 300
 REMARK 300 THE PROTEIN IS A HOMODIMER FORMED BY CHAIN A.
 REMARK 300 A HETERODIMERIC ASSOCIATION OF CHAIN A WITH CHAIN S
 REMARK 300 PRODUCES A TETRAMER.
 REMARK 300
 REMARK 300 THE BURIED SURFACE AREA SHOWN BELOW IS AN AVERAGE
 REMARK 300 CALCULATED FOR THE HETEROTETRAMER AND DOES NOT
 REMARK 300 CORRESPOND TO THE BURIED SURFACE AREA FOR THE .
 REMARK 300 HOMODIMER OF CHAIN A
 REMARK 300
 REMARK 300 THE HETERO-ASSEMBLY DESCRIBED BY REMARK 350 APPEARS
  REMARK 300 TO BE A CASE OF STRONG CRYSTAL PACKING WITH
  REMARK 300 THE MEAN DIFFERENCE IN ACCESSIBLE SURFACE AREA PER
  REMARK 300 CHAIN BETWEEN THE ISOLATED CHAIN AND THAT FOR
  REMARK 300 THE CHAIN IN THE COMPLEX IS 2149.4 ANGSTROM**2
  REMARK 350
  REMARK 350 GENERATING THE BIOMOLECULE
  REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
  REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
  REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
  REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND
  REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
  REMARK 350
  REMARK 350 BIOMOLECULE: 1
  REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, S
  REMARK 350 BIOMT1 1 1.000000 0.000000 0.000000
                                                                             0.00000
```

```
0.00000
             BIOMT2
                          0.000000
                                    1.000000
                                                0.000000
REMARK 350
                       1
                                                1.000000
                                                                  0.00000
             BIOMT3
                          0.000000
                                    0.000000
REMARK 350
                       1
                                                                86.24900
                                                0.000000
             BIOMT1
                       2 0.000000 -1.000000
REMARK 350
                                                                86.24900
                       2 -1.000000
                                     0.000000
                                                0.000000
REMARK 350
             BIOMT2
REMARK 350
             BIOMT3
                           0.000000
                                     0.000000 - 1.000000
                                                                74.13000
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
              M RES C SSSEQI
REMARK 465
                MET A
REMARK 465
                           1
                ALA A
                           2
REMARK 465
                           3
                ALA A
REMARK 465
                THR A
                           4
REMARK 465
                           5
REMARK 465
                ALA A
REMARK 465
                ALA A
                           6
REMARK 465
                GLU A
                           7
REMARK 465
                ALA A
                           8
REMARK 465
                VAL A
                           9
                ALA A
                          10
REMARK 465
                SER A
REMARK 465
                          11
REMARK 465
                GLY A
                          12
REMARK 465
                SER A
                          13
REMARK 465
                GLY A
                          14
REMARK 465
                LYS A
                         304
REMARK 465
                ARG A
                         305
REMARK 465
                ILE A
                         306
REMARK 465
                PRO S
                         775
                SER S
REMARK 465
                         776
                ASP S
                         777
REMARK 465
REMARK 465
                LEU S
                         778
REMARK 465
                 ALA S
                         779
                 CYS S
                         780
 REMARK 465
                 ARG S
 REMARK 465
                         781
                 LEU S
 REMARK 465
                         782
 REMARK 465
                 LEU S
                         783
 REMARK 465
                 GLY S
                         784
 REMARK 465
                 GLN S
                         785
 REMARK 465
                 SER S
                         786
                 MET S
 REMARK 465
                         787
                 ASP S
 REMARK 465
                         788
 REMARK 465
                 GLU S
                         789
 REMARK 465
                 SER S
                         790
 REMARK 465
                 GLY S
                         791
 REMARK 465
                 LEU S
                         792
 REMARK 465
                 PRO S
                         793
                 GLN S
 REMARK 465
                          794
                 GLN S
 REMARK 465
                          807
                 GLY S
 REMARK 465
                          808
 REMARK 465
                 SER S
                          809
 REMARK 465
                 ARG S
                          810
 REMARK 465
                 ASN S
                          811
 REMARK 465
                 LEU S
                          812
 REMARK 465
                 ASP S
                          823
                 GLN S
                          824
 REMARK 465
 REMARK 465
                 VAL S
                          825
 REMARK 465
                 ASN S
                          826
 REMARK 470
 REMARK 470 MISSING ATOM
```

```
REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;
REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;
REMARK 470 I=INSERTION CODE):
REMARK 470
             M RES CSSEQI ATOMS
               GLU A 15
GLU A 29
ASN A 87
REMARK 470
                            CG
                                 CD
                                       OE1
                                            OE2
                            CG
                                 CD
                                       OE1
                                            OE2
REMARK 470
REMARK 470
                            CG
                                 OD1
                                      ND2
               LYS A 106
REMARK 470
                            CD
                                 CE
                                       NZ
REMARK 470
               LYS A 115
                            CG
                                  CD
                                       CE
                                            NZ
REMARK 470
               ARG A 117
                            CG
                                  CD
                                       NE
                                            CZ
                                                 NH1 NH2
REMARK 470
              GLN A 133
                            CG
                                  CD
                                       OE1
                                            NE2
              GLN A 136
                            CG
                                       OE1
                                            NE2
REMARK 470
                                  CD
REMARK 470
                                            NE2
               GLN A 137
                            CG
                                  CD
                                       OE1
               ARG A 156
                            CG
                                  CD
                                       NE
                                            CZ
                                                 NH1 NH2
REMARK 470
REMARK 470
               LYS A 157
                            CD
                                  CE
                                       NZ
                                            NZ
REMARK 470
                                       CE
               LYS A 311
                            CG
                                  CD
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 3(1X, A4, 2X), 12X, F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500
            M RES CSSEQI ATM1
                               ATM2
                                        ATM3
               LEU A 227
                         CA - CB - CG ANGL. DEV. = -11.0 DEGREES
REMARK 500
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD AND BY MORE THAN 0.150 ANGSTROMS (M=MODEL
 REMARK 500 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
 REMARK 500 NUMBER; I=INSERTION CODE).
 REMARK 500
 REMARK 500 STANDARD TABLE:
 REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 1X, 2(A4, A1, 3X), 12X, F5.3)
 REMARK 500
 REMARK 500 EXPECTED VALUESS: ENGH AND HUBER, 1991
 REMARK 500
                                                    DEVIATION
 REMARK 500
             M RES CSSEQI ATM1
                                 RES CSSEQI ATM2
 REMARK 500
               MET A 343 SD
                                  MET A 343 CE
                                                     -0.209
 REMARK 500
 REMARK 500 REMARK: NULL
 REMARK 500
 REMARK 500 GEOMETRY AND STEREOCHEMISTRY
 REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
 REMARK 500
 REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
 REMARK 500
                                  ATM2 RES C SSEQI
 REMARK 500
             ATM1 RES C SSEQI
                                                                 DISTANCE
 REMARK 500
```

```
REMARK 500 · O
                 ALA A
                          300
                                  OH
                                       TYR S
                                               798
                                                                 2.09
REMARK 525
REMARK 525 SOLVENT
REMARK 525
REMARK 525 THE SOLVENT MOLECULES ARE GIVEN CHAIN IDENTIFIERS TO
REMARK 525 INDICATE THE PROTEIN CHAIN TO WHICH THEY ARE MOST CLOSELY
REMARK 525 ASSOCIATED WITH:
             PROTEIN CHAIN SOLVENT CHAIN
REMARK 525
REMARK 525
                              Z
               Α
REMARK 525
                              Н
REMARK 600
REMARK 600 HETEROGEN
REMARK 600
REMARK 600 FOR METAL ATOM ZN
                                ZN A1350 THE COORDINATION ANGLES ARE:
           1 HIS
                    199A NE2
REMARK 600
REMARK 600
            2 ASP
                    201A
                         OD2
                                    103.4
           3 HIS
REMARK 600
                    279A NE2
                                    .84.2
                                           88.5
REMARK 600
           4 OGA
                  1351A O2
                                    169.0 87.2
                                                 99.0
REMARK 600 5 OGA 1351A 02'
                                   86.3 169.1 97.3
                                                       82.8
REMARK 600
                                       1
                                             2
                                                   3
REMARK 700
REMARK 700 SHEET
REMARK 700 THE SHEET STRUCTURE OF THIS MOLECULE IS BIFURCATED. IN
REMARK 700 ORDER TO REPRESENT THIS FEATURE IN THE SHEET RECORDS BELOW,
REMARK 700 TWO SHEETS ARE DEFINED.
REMARK 800
REMARK 800 SITE
REMARK 800 SITE IDENTIFIER: ZNA
REMARK 800 SITE DESCRIPTION: ZN BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE IDENTIFIER: OGA
REMARK 800 SITE DESCRIPTION: OGA BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE IDENTIFIER: SA1
REMARK 800 SITE DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE IDENTIFIER: SA2
REMARK 800 SITE DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 1D7G
                              RELATED DB: PDB
REMARK 900 A MODEL FOR THE COMPLEX BETWEEN THE
REMARK 900 . HYPOXIA-INDUCIBLE FACTOR-1 (HIF-1) AND ITS
REMARK 900
             CONSENSUS DEOXYRIBONUCLEIC ACID SEQUENCE
REMARK 900 RELATED ID: 1H2K
                             RELATED DB: PDB
 REMARK 900
            FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
 REMARK 900
            WITH HIF-1 ALPHA FRAGMENT PEPTIDE
 REMARK 900 RELATED ID: 1H2L
                              RELATED DB: PDB
 REMARK 900
            FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
 REMARK 900
            WITH HIF-1 ALPHA FRAGMENT PEPTIDE
 REMARK 900 RELATED ID: 1H2N
                             RELATED DB: PDB
 REMARK 900
            FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
 REMARK 900
            WITH HIF-1 ALPHA FRAGMENT PEPTIDE
 REMARK 900 RELATED ID: 1L8C
                             RELATED DB: PDB
            STRUCTURAL BASIS FOR HIF-1ALPHA/CBP
 REMARK 900
            RECOGNITION IN THECELLULAR HYPOXIC RESPONSE
 REMARK 900
 REMARK 900 RELATED ID: 1LM8
                              RELATED DB: PDB
 REMARK 900 STRUCTURE OF A HIF-1A-PVHL-ELONGINB-
 REMARK 900 ELONGINC COMPLEX
 REMARK 900 RELATED ID: 1LQB
                               RELATED DB: PDB
```

REMARK 900 CRYSTAL STRUCTURE OF A HYDROXYLATED HIF-1

```
REMARK 900 ALPHA PEPTIDEBOUND TO THE PVHL/ELONGIN-C/
REMARK 900 ELONGIN-B COMPLEX
                                                                   349
                                  Q969Q7
                                           Q969Q7
                 1
                     349 SWS
       1H2M A
DBREF
                                           HIFA HUMAN
                     826 SWS
                                  Q16665
       1H2M S
              775
              349 MET ALA ALA THR ALA ALA GLU ALA VAL ALA SER GLY SER
         1 A
SEORES
                   GLY GLU PRO ARG GLU GLU ALA GLY ALA LEU GLY PRO ALA
SEORES
              349
                    TRP ASP GLU SER GLN LEU ARG SER TYR SER PHE PRO THR
              349
SEORES
                    ARG PRO ILE PRO ARG LEU SER GLN SER ASP PRO ARG ALA
              349
SEORES
         4 A
                    GLU GLU LEU ILE GLU ASN GLU GLU PRO VAL VAL LEU THR
SEQRES
              349
         5 A
                    ASP THR ASN LEU VAL TYR PRO ALA LEU LYS TRP ASP LEU
         6 A
              349
SEQRES
                    GLU TYR LEU GLN GLU ASN ILE GLY ASN GLY ASP PHE SER
         7 A
              349
SEQRES
                    VAL TYR SER ALA SER THR HIS LYS PHE LEU TYR TYR ASP
SEQRES
         8 A
              349
                    GLU LYS LYS MET ALA ASN PHE GLN ASN PHE LYS PRO ARG
         9 A
              349
SEQRES .
                    SER ASN ARG GLU GLU MET LYS PHE HIS GLU PHE VAL GLU
              349
        10 A
SEQRES
                    LYS LEU GLN ASP ILE GLN GLN ARG GLY GLY GLU GLU ARG
              349
        11 A
SEQRES
                    LEU TYR LEU GLN GLN THR LEU ASN ASP THR VAL GLY ARG
        12 A
              349
SEQRES
                    LYS ILE VAL MET ASP PHE LEU GLY PHE ASN TRP ASN TRP
               349
        13 A
SEQRES
                    ILE ASN LYS GLN GLN GLY LYS ARG GLY TRP GLY GLN LEU
               349
SEQRES
        14 A
                    THR SER ASN LEU LEU LEU ILE GLY MET GLU GLY ASN VAL
SEORES
         15 A
               349
                    THR PRO ALA HIS TYR ASP GLU GLN GLN ASN PHE PHE ALA
SEQRES
         16 A
               349
                    GLN ILE LYS GLY TYR LYS ARG CYS ILE LEU PHE PRO PRO
               349
SEQRES
         17 A
                    ASP GLN PHE GLU CYS LEU TYR PRO TYR PRO VAL HIS HIS
               349
SEQRES
         18 A
                    PRO CYS ASP ARG GLN SER GLN VAL ASP PHE ASP ASN PRO
 SEQRES
         19 A
               349
                    ASP TYR GLU ARG PHE PRO ASN PHE GLN ASN VAL VAL GLY
 SEORES
         20 A
               349
                    TYR GLU THR VAL VAL GLY PRO GLY ASP VAL LEU TYR ILE
 SEORES
         21 A
               349
                    PRO MET TYR TRP TRP HIS HIS ILE GLU SER LEU LEU ASN
 SEQRES
         22 A
               349
                    GLY GLY ILE THR ILE THR VAL ASN PHE TRP TYR LYS GLY
 SEQRES
         23 A
               349
                    ALA PRO THR PRO LYS ARG ILE GLU TYR PRO LEU LYS ALA
         24 A
               349
 SEQRES
                    HIS GLN LYS VAL ALA ILE MET ARG ASN ILE GLU LYS MET
         .25 A
               349
 SEQRES
                    LEU GLY GLU ALA LEU GLY ASN PRO GLN GLU VAL GLY PRO
               349
 SEQRES
         26 A
                    LEU LEU ASN THR MET ILE LYS GLY ARG TYR ASN
 SEQRES
         27 A
               349
                     PRO SER ASP LEU ALA CYS ARG LEU LEU GLY GLN SER MET
 SEQRES
          1 S
                52
                     ASP GLU SER GLY LEU PRO GLN LEU THR SER TYR ASP CYS
 SEQRES
          2 S
                 52
                     GLU VAL ASN ALA PRO ILE GLN GLY SER ARG ASN LEU LEU
          3 S
                 52
 SEQRES
                     GLN GLY GLU GLU LEU LEU ARG ALA LEU ASP GLN VAL ASN
 SEQRES
          4 S
                 52
         ZN
            A1350
                          1
 HET
        OGA A1351
 HET
                         10
 HET
        SO4
             A1352
                          5
             A1353
 HET
        SO4
              ZN ZINC ION
 HETNAM
             OGA N-OXALYOLGLYCINE
 HETNAM
             SO4 SULFATE ION
 HETNAM
           3
              ZN
                     ZN1 2+
 FORMUL
              OGA .
                     C4 H5 N1 O5
 FORMUL
           4
 FORMUL
           5
              SO4
                     2(04 $1 2-)
                   *99(H2 O1)
           6
              HOH
 FORMUL
                                                                                5
                                      32
                                          5
               1 ASP A
                         28
 HELIX
           1
                             LEU A
                                                                               10
                                      58
                                          1
           2
                          49
                             ASN A
 HELIX
               2 ASP A
                                                                                7
                         70
                              TRP A
                                      76
                                          5
           3
               3 VAL A
 HELIX
                                                                                9
           4
               4 ASP A
                         77
                              ILE A
                                      85
                                          1
 HELIX
                                                                                9
  HELIX
           5
               5 ASP A
                        104
                              GLN A
                                     112
                                          5
                                                                               15
                                          1
  HELIX
           6
               6 LYS A
                        124
                              ARG A
                                     138
                                                                                10
                        155
                              GLY A
                                     164
                                          1
  HELIX
           7
               7 GLY A
                                                                                12
                              ARG A
                                     177
  HELIX
           8
               8 · ASN A
                        166
                                                                                 3
                                     222
                              ASP A
                                           5
           9
               9 PRO A
                         220
  HELIX
                                                                                 6
              10 GLN A
                         223
                              TYR A
                                     228
          10
  HELIX
                                                                                 7
                         252
                              VAL A
                                     258
                                           5
              11 PHE A
  HELIX
          11
                                                                                21
                         311
          12
              12 LYS A
                              GLY A
                                     331
  HELIX
                                                                                 3
                                           5
                         332
                              GLN A
                                     334
          13
              13 ASN A
  HELIX
                                                                                11
                                           1
                         335
                              LYS A
                                     345
  HELIX
          14
              14 GLU A
                                                                                 9
              15 GLN S
                        814
                              LEU S 822
          15
  HELIX
```

SHEET	1 AA 5 THR A 39 PRO A 41 0	
SHEET	2 AA 5 GLY A 260 VAL A 265 1 O GLY A 260 N ARG A 40	
SHEET	3 AA 5 LYS A 214 PHE A 219 -1 O LYS A 214 N VAL A 265	
SHEET	4 AA 5 TRP A 278 SER A 283 -1 O TRP A 278 N PHE A 219	
SHEET	5 AA 5 VAL A 195 HIS A 199 -1 O THR A 196 N ILE A 281	
SHEET	1 AB 6 ARG A 44 LEU A 45 0	
SHEET	2 AB 6 VAL A 62 LEU A 64 1 O VAL A 63 N LEU A 45	
SHEET	3 AB 6 VAL A 270 ILE A 273 -1 O VAL A 270 N LEU A 64	
SHEET	4 AB 6 GLN A 203 LYS A 211 -1 O ASN A 205 N ILE A 273	
SHEET		
SHEET	6 AB 6 LEU A 182 SER A 184 -1 N THR A 183 O TRP A 296	
SHEET	1 AC 9 ARG A 44 LEU A 45 0	
SHEET	2 AC 9 VAL A 62 LEU A 64 1 O VAL A 63 N LEU A 45	
SHEET	3 AC 9 VAL A 270 ILE A 273 -1 O VAL A 270 N LEU A 64	
SHEET	4 AC 9 GLN A 203 LYS A 211 -1 O ASN A 205 N ILE A 273	
SHEET	5 AC 9 THR A 290 LYS A 298 -1 O ILE A 291 N ILE A 210	
SHEET	6 AC 9 LEU A 186 GLY A 190 -1 O LEU A 186 N ASN A 294	
SHEET	7 AC 9 ARG A 143 .THR A 149 -1 O LEU A 146 N ILE A 189	
SHEET	8 AC 9 PHE A 90 ALA A 95 -1 O SER A 91 N GLN A 147	
SHEET	9 AC 9 SER A 118 MET A 123 -1 O ASN A 119 N SER A 94	
LINK	ZN ZN A1350 NE2 HIS A 199 1555 1555	
LINK	ZN ZN A1350 OD2 ASP A 201 1555 1555	
LINK	ZN ZN A1350 NE2 HIS A 279 1555 1555	
LINK	ZN ZN A1350 O2 OGA A1351 1555 1555	
LINK	ZN ZN A1350 O2' OGA A1351 1555 1555	
CISPEP	1 TYR A 308 PRO A 309 0 1.05	
SITE	1 ZNA 3 HIS A 199 ASP A 201 HIS A 279	
SITE		
SITE	2 OGA 13 ASP A 201 ASN A 205 PHE A 207 LYS A 214	
SITE	3 OGA 13 HIS A 279 ILE A 281 ASN A 294 TRP A 296	
SITE	4 OGA 13 HOH Z 47	
SITE	1 SA1 4 ARG A 138 GLY A 140 GLU A 141 GLU A 142	
SITE	1 SA2 5 ARG A 143 GLU A 192 GLY A 193 LEU A 285	
SITE	2 SA2 5 ASN A 286	
CRYST1	86.249 86.249 148.260 90.00 90.00 90.00 P 41 21 2 8	
ORIGX1	1.000000 0.000000 0.000000 0.00000	
ORIGX2	0.000000 1.000000 0.000000 0.00000	
ORIGX3	0.000000 0.000000 1.000000 0.00000	
SCALE1	0.011594 0.000000 0.000000 0.00000	
SCALE2	0.000000 0.011594 0.000000 0.00000	
SCALE3	0.000000 0.000000 0.006745 0.00000	
ATOM	1 N GLU A 15 8.462 32.732 9.880 1.00 78.57	N
ATOM	2 CA GLU A 15 7.114 32.108 9.773 1.00 78.75	C
MOTA	3 C GLU A 15 7.207 30.654 10.192 1.00 78.42	С
MOTA	4 O GLU A 15 8.067 29.928 9.714 1.00 78.63	0
ATOM	5 CB GLU A 15 6.580 32.219 8.345 1.00 78.95	С
· ATOM	6 N PRO A 16 6.316 30.214 11.067 1.00 78.20	N
ATOM	7 CA PRO A 16 6.376 28.840 11.584 1.00 77.89	C
ATOM	8 C PRO A 16 6.328 27.796 10.467 1.00 77.35	č
ATOM	9 O PRO A 16 5.541 27.888 9.527 1.00 76.95	ŏ
MOTA	10 CB PRO A 16 5.146 28.746 12.493 1.00 78.00	c
		C
ATOM		
ATOM	12 CD PRO A 16 5.173 30.969 11.605 1.00 78.24	C
ATOM	13 N ARG A 17 7.184 26.796 10.580 1.00 76.88	N
ATOM	14 CA ARG A 17 7.264 25.749 9.575 1.00 76.63	C
ATOM	15 C ARG A 17 6.005 24.891 9.539 1.00 75.45	С
MOTA	16 O ARG A 17 5.247 24.836 10.505 1.00 75.40	0
ATOM	17 CB ARG A 17 8.444 24.820 9.875 1.00 77.06	С
ATOM	18 CG ARG A 17 9.816 25.481 9.900 1.00 78.68	С
MOTA	19 CD ARG A 17 10.954 24.522 10.293 1.00 80.53	С
MOTA	20 NE ARG A 17 10.908 24.086 11.699 1.00 82.60	N

									1 00 04 07	
ATOM	21		ARG A		17	11.401	24.776	12.744	1.00 84.27	
ATOM	22		ARG A		17	11.980	25.968	12.584	1.00 83.33	
MOTA	23		ARG A		17	11.311	24.268	13.967	1.00 85.10	
MOTA	24		GLU A		18	5.796	24.209	8.421	1.00 74.01	
MOTA	25		GLU A		18	4.692	23.274	8.319	1.00 72.99	
MOTA	26		GLU A		18	5.193	21.855	8.607	1.00 71.43	
MOTA	27	0	GLU A	7	18	6.210	21.421	8.061	1.00 70.71	
ATOM	28	CB	GLU A	1	18	4.033	23.352	6.938	1.00 73.29	
ATOM	29	CG	GLU P	1	18 ·	3.333	24.677	6.659	1.00 73.91	
ATOM	30	CD	GLU F	Ą	18	1.949	24.794	7.283	1.00 74.30	
ATOM	31	OE1	GLU. P	A	18	1.355	23.776	7.692	1.00 74.07	
ATOM	32	OE2	GLU F	Ą	18	1.444	25.929	7.356	1.00,75.76	
MOTA	33	N	GLU A	Ą	19	4.482	21.157	9.491	1.00 69.89	
MOTA	34	ÇA	GLU A	Ą	19	4.786	19.764	9.818	1.00 68.89	
ATOM	35	С	GLU A	Ą	19	4.393	18.854	8.661	1.00 66.65	
MOTA	36		GLU I		19	3.324	19.011	8.065	1.00 65.92	
ATOM	37		GLU Z		19	4.058	19.311	11.096	1.00 69.41	
ATOM	38	CG	GLU A		19	4.544	19.996	12.370	1.00 72.06	
ATOM	39	CD	GLU Z		19	4.308	19.194	13.657	1.00 76.41	
ATOM	40		GLU Z		19	3.855	18.016	13.609	1.00 78.21	
MOTA	41		GLU Z		19	4.590	19.758	14.746	1.00 79.64	
ATOM	42	N	ALA		20	5.283	17.919	8.349	1.00 64.54	
ATOM	43	CA	ALA .		20	5.067	16.921	7.303	1.00 63.03	
ATOM	44	C	ALA		20	3.735	16.225	7.449	1.00 61.23	
ATOM	45	Ö	ALA		20	3.303	15.903	8.556	1.00 60.61	
ATOM	46	СВ	ALA		20	6.177	15.889	7.312	1.00 62.82	
ATOM	47	И	GLY		21	3.087	16.002	6.316	1.00 59.29	
ATOM	48	CA	GLY		21	1.833	15.289	6.304	1.00 58.26	
	49	C	GLY		21	0.651	16.200	6.530	1.00 57.44	
ATOM		0	GLY		21	-0.416	15.739	6.873	1.00 56.42	
MOTA	50		ALA		22	0.858	17.500	6.341	1.00 57.28	
ATOM	51				22	-0.182	18.509	6.492	1.00 56.92	
ATOM	52	CA	ALA		22	-0.737	18.544	7.909	1.00 56.53	
ATOM	53	C .	ALA			-1.926		8.108	1.00 56.32	
MOTA	54		ALA		22			5.488	1.00 57.10	
MOTA	55		ALA		22	-1.285		8.898	1.00 56.25	
ATOM	56		LEU		23	0.133		10.289	1.00 56.23	
ATOM	57		LEU		23	-0.306		10.283	1.00 55.03	
ATOM	58		LEU		23	-0.385			1.00 54.89	•
ATOM	59		LEU		23	-0.638			1.00 56.05	
ATOM	60		LEU		23	0.583	•		1.00 58.05	
MOTA	61	CG	LEU	A	23	0.445		10.678	1.00 58.00	
MOTA	62		LEU		23	1.307				
MOTA	63		LEU		23	-1.030			1.00 59.53	
MOTA	. 64		GLY		24	-0.202				
MOTA	65		GLY		24	-0.337			1.00 53.43	
MOTA	66		GLY		24	0.932			1.00 52.71	
MOTA	67		GLY		24	2.025			1.00 52.28	
MOTA	68		PRO		25 -	0.775			1.00 51.60	
MOTA	69	CA	PRO		25	1.908				
ATOM	70) C	PRÓ		25	2.310				
MOTA	71	LO	PRO	Α	25	1.481				
MOTA	72		PRO			1.366				
MOTA	73	G CG	PRO	A		-0.109				
MOTA	. 74		PRO	A	25	-0.493				
ATOM	7		ALA			3.616				
ATOM	7		ALA			4.218				
ATOM	7		ALA			3.894				
ATOM	7		ALA			3.64		16.836		
ATOM	7					5.71		14.328		
ATOM	-8		TRP			3.86			1.00 45.91	
ATOM	8					3.49				
	•					-				

ATOM	82	С	TRP 2		27	3.003	27.818	16.107	1.00 44.47	С
MOTA	83	0	TRP .		27	2.985	27.981	14.901	1.00 44.30	0
ATOM	84	CB	TRP .		27	4.719	26.727	17.568	1.00 44.91	С
ATOM	85	CG	TRP .		27	5.916	26.910	16.737	1.00 42.67	С
MOTA	86		TRP .		27	6.702	25.934	16.197	1.00 43.38	С
MOTA	87		TRP		27	6.411	28.129	16.255	1.00 38.70	. C
ATOM	88		TRP		27	7.690	26.494	15.425	1.00 41.56	N
ATOM	89		TRP		27	7.532	27.847	15.452	1.00 39.59	C
ATOM	90		TRP		27	6.039	29.442	16.431 14.861	1.00 38.28	C C
ATOM	91	CZ2 CZ3	TRP		27	8.284	28.827		1.00 39.74	C
ATOM ATOM	92 93		TRP TRP		27 27	6.781 7.884	30.409 30.104	15.849 15.057	1.00 39.48 1.00 40.17	C
ATOM	94	N	ASP		28	2.580	28.760	16.941	1.00 43.91	N
ATOM	95	CA	ASP		28	2.230	30.079	16.417	1.00 43.91	C
ATOM	96	C	ASP		28	2.750	31.161	17.305	1.00 43.07	C.
ATOM	97	Ö	ASP		28	3.191	30.901	18.409	1.00 42.11	ŏ
MOTA	98	СВ	ASP		28	0.722	30.251	16.199	1.00 44.82	Č
ATOM	99	CG	ASP		28	-0.052	30.162	17.462	1.00 47.87	Ċ
ATOM	100		ASP		28	-0.240	31.236	18.108	1.00 50.91	0
ATOM	101		ASP		28	-0.501	29.054	17.877	1.00 49.06	0
MOTA	102	N	GLU		29	2.713	32.385	16.790	1.00 41.29	N
ATOM	103	CA	GLU	Α	29	3.208	33.586	17.499	1.00 39.69	С
ATOM	104	С	GLU	Α	29	2.685	33.711	18.917	1.00 37.94	С
MOTA	105	0	GLU	A	29	3.415	34.069	19.801	1.00 37.26	0
ATOM	106	CB	GLU	Α	29	2.840	34.812	16.735	1.00 39.59	С
MOTA	107	N	SER		30	1.427	33.371	19.135	1.00 36.78	N
ATOM	108	CA	SER		30	0.810	33.558	20.443	1.00 36.13	С
MOTA	109	С	SER		30	1.501	32.756	21.517	1.00 35.30	С
ATOM	110	0	SER		30	1.252	32.968	22.678	1.00 35.21	0
ATOM	111	CB	SER		30	-0.686	33.180	20.406	1.00 35.84	C
ATOM	112	OG	SER		30	-0.901	31.762	20.450	1.00 36.93	0
MOTA	113	N	GLN		31	2.326	31.795	21.116	1.00 35.24	N
ATOM	114	CA	GLN		31	3.021	30.918	22.060	1.00 34.89	C
ATOM	115	C	GLN		31	4.366	31.506	22.487 23.365	1.00 34.60	C 0
ATOM ATOM	116 117	O CB	GLN GLN		31 31	5.010 3.224	30.969 29.513	21.473	1.00 34.18 1.00 34.65	c
ATOM	118	CG	GLN		31	1.969	28.649	21.402	1.00 34.03	C
MOTA	119	CD	GLN		31	2.212	27.322	20.707	1.00 34.74	c
ATOM	120	0E1			31	2.215	27.249	19.476	1.00 32.57	Ö
MOTA	121	NE2			31	2.442	26.278	21.492		N
MOTA	122	N	LEU		32	4.753		21.895	1.00 34.85	N
ATOM	123	CA	LEU		32	6.016		22.212	1.00 35.01	C
ATOM	124	C	LEU		32	5.798		23.223	1.00 34.91	· C
MOTA	125	0	LEU		32	4.834		23.125	1.00 35.83	0
MOTA	126	CB	LEU	Α	32	6.631		20.945	1.00 34.96	С
MOTA	127	CG	LEU	Α	32	6.995	32.860	19.849	1.00 36.03	С
MOTA	128	CD1	LEU	Α	32	7.691	33.525	18.701	1.00 36.15	С
MOTA	129	CD2	LEU	Α	32	7.855	31.780	20.377	1.00 35.18	С
MOTA	130	N	ARG		33	6.675		24.209	1.00 34.49	N
ATOM	131	CA	ARG		33	6.564		25.170	1.00 34.33	C
ATOM	132	C	ARG		33	7.005		24.460	1.00 34.37	С
ATOM	133	0	ARG		33	7.733		23.498	1.00 34.87	0
MOTA	134	CB	ARG		33	7.442		26.394	1.00 34.16	C
MOTA	135	CG	ARG		33	7.056		27.212	1.00 32.83	C
ATOM	136	CD	ARG		33	7.951		28.428	1.00 33.34	C
ATOM	137	NE	ARG		33	7.413		29.252	1.00 34.91	N
ATOM	138	CZ	ARG		33	6.445		30.137	1.00 36.53	C
MOTA	139		ARG		33	5.900		30.382	1.00 34.89	N
MOTA	140		ARG		33	6.027		30.795	1.00 39.39	N
MOTA	141	N	SER		34 34	6.608 6.944		24.947	1.00 34.36	N
MOTA	142	CA	SER	. A	54	0.944	39.247	24.244	1.00 34.69	С

M	140		a E D	70	24		8.002	40.055	24.987	1.00 33.26	C	•
	143	_	SER		34 34		7.958	40.033	26.200	1.00 33.20		5
MO:	144	O	SER SER		34		5.698	40.192	24.143	1.00 35.33		Ĉ
MO	145	CB	SER		34		5.586	40.744	25.393	1.00 39.99		5
MOJ	146 147	og N	TYR		35		8.911	40.682	24.252	1.00 32.38		N
[Ozzi	148	CA	TYR		35		10.080	41.329	24.843	1.00 32.03		C
MOJ	149	C	TYR		35		10.339	42.675	24.193	1.00 32.52		С
rom	150	ŏ	TYR		35		9.763	42.979	23.172	1.00 32.78		0
COM	151	СВ	TYR	-	35		11.290	40.422	24.686	1.00 31.20	Ċ	C
ГОМ	152	CG	TYR		35	•	11.139	39.161	25.482	1.00 30.69		С
ГОМ	153	CD1	TYR		35		10.935	39.215	26.853	1.00 30.40		С
rom	154	CD2	TYR	Α	35		11.186	37.915	24.875	1.00 30.34		С
MOT	155	CE1	TYR	Α	35		10.804	38.054	27.609	1.00 31.74		С
MO1	156	CE2	TYR	Α	35		11.050	36.741	25.617	1.00 32.05		С
MOT	157	CZ	TYR		35		10.858	36.812	26.991	1.00 31.98		C
rom	158	OH	TYR		35		10.687	35.658	27.742	1.00 30.13		0
MOI	159	N	SER		36		11.240	43.463	24.761	1.00 33.06		N
TOM	160	CA	SER		36		11.469	44.838	24.289	1.00 32.95		C C
TOM	161	С	SER		36		12.469	44.977	23.159	1.00 32.65 1.00 33.04		0
TOM	162	0	SER		36		12.705	46.084	22.674	1.00 33.04		C
TOM	163	CB	SER		36		11.979	45.698 45.325	25.438 25.844	1.00 32.92		0
TOM	164	OG	SER		· 36 37		13.272 13.041	43.323	22.711	1.00 33.03		N
TOM TOM	165 166	N CA	PHE PHE		37		14.100	43.988	21.740	1.00 31.55		C
TOM	167	C	PHE		37		13.784	43.269	20.444	1.00 31.69		c
TOM	168	Ö	PHE		37		13.020	42.326	20.386	1.00 32.65		0
TOM	169	СВ	PHE		37		15.421	43.431	22.339	1.00 30.68		С
TOM	170		PHE		37		15.275	42.054	22.890	1.00 30.10		C
TOM	171		PHE		37		15.329		22.060	1.00 28.43		С
MOT	172		PHE		37		15.022	41.852	24.231	1.00 29.43		С
.TOM	173	CE1	PHE	A	37		15.168	39.679	22.564	1.00 31.59		С
MOT.	174	CE2	PHE	Α	37		14.852	40.580	24.733	1.00 30.52		С
MOT.	175	CZ	PHE		37		14.927	39.495	23.915	1.00 31.81		С
MOT.	176	N	PRC		38		14.403	43.721	19.384	1.00 31.70		N.
. MOT.	177	CA	PRC		38		14.268	43.036	18.106	1.00 31.23		С
MOT.	178	C	PRC		38		15.231	41.895	17.984	1.00 31.71		. C
MOŢ.	179	0	PRC		38		16.205	41.880	18.743	1.00 31.59		0 C
MOT.	180	CB	PRO		38		14.652	44.118	17.117	1.00 31.44 1.00 32.43		C
MOT.	181	CG	PRO		38 38		15.636 15.186	45.005 44.973	17.922 19.320	1.00 32.43		C
MOT.	182 183	CD N	PRC THE				14.996	41.008	17.003	1.00 30.20		N
MOT. MOT.	184	CA	THE				15.868	39.891	16.702	1.00 32.00	• •	Ċ
MOT	185	C	THE				15.865	39.606	15.203	1.00 32.89		C
MOT	186	Ö	THE				14.998	40.048	14.476	1.00 32.28		0
MOT	187	СВ		RA			15.370	38.647	17.377	1.00 32.26		С
MOT	188	OG:					14.024	38.389	16.949	1.00 30.59		0
MOT	189		2 THE				15.235	38.832	18.905	1.00 32.99		С
MOTA	190	N	AR	G A	40		16.855	38.844	14.770	1.00 33.28		Ν.
MOT2	191	CA	AR	G A	40		16.980	38.372	13.421	1.00 34.30		С
MOTA	192	С		G A			17.023			1.00 33.77		С
MOTA	193	0		G A			17.288			1.00 34.68		0
MOT!	194	CB		G A			18.267			1.00 34.73		C
MOTA	195			G A			18.273					C
MOTA	196			G A			16.909			1.00 48.38		C
MOTA	197			G A			16.728					N C
MOTA	198			G A			15.553					И
MOTA	199		1 AR				14.501 15.415					N
MOT!	200 201		2 AR	G P			16.663					N
MOTA	201			O F			16.646					C
MOTA	202			O P			18.002					Ċ
11013	د ن	•	* 1/	. · ·	. 41		10.002	54.010	,,			_

ATOM	204	0	PRO	A	41	18.907	34.475	11.801	1.00 34.64	o
ATOM	205	CB	PRO		41	15.800	34.299	11.340	1.00 33.22	C
MOTA	206	CG	PRO		41	15.409	35.563	10.675	1.00 33.55	C
MOTA	207	CD	PRO		41	16.038	36.717	11.343	1.00 32.95	C
ATOM	208	N	ILE		42	18.154	32.925	13.192	1.00 30.97	N
ATOM	209	CA	ILE		42	19.337	32.144	13.049	1.00 29.87	C
ATOM	210	C	ILE		42	19.077	31.289	11.814	1.00 30.07	C
ATOM	211	0	ILE		42	17.946	30.857	11.587	1.00 30.17	0
ATOM ATOM	212 213	CB	ILE		42	19.477	31.306	14.273	1.00 29.85	C
ATOM	214	CG1 CG2	ILE		42 42	19.721	32.215	15.478	1.00 27.79	C
ATOM	215	CD1				20.582	30.264	14.105	1.00 30.60	C
ATOM	216	И	ILE PRO		42 43	19.565	31.503	16.788	1.00 25.35	C
ATOM	217	CA	PRO		43	20.085 19.922	31.075 30.219	10.985 9.823	1.00 29.34 1.00 29.60	N
ATOM	218	C	PRO		43	19.623	28.751	10.176	1.00 29.60	C
ATOM	219	ō	PRO		43	20.207	28.265	11.160	1.00 30.63	. C
ATOM	220	СВ	PRO		43	21.288	30.310	9.139	1.00 30.00	. C
ATOM	221	CG	PRO		43	21.933	31.491	9.665	1.00 28.87	c
ATOM	222	CD	PRO		43	21.420	31.676	11.047	1.00 28.76	c
ATOM	223	N	ARG		44	18.725	28.103	9.419	1.00 30.34	N
MOTA	224	CA	ARG		44	18.415	26.693	9.507	1.00 31.59	C
MOTA	225	C .	ARG		44	18.965	26.050	8.267	1.00 31.44	c
ATOM	226	0	ARG		44	18.540	26.359	7.169	1.00 32.24	ō
MOTA	227	CB	ARG	Α.	44	16.923	26.399	9.502	1.00 32.07	Ċ
MOTA	228	CG	ARG	A	44	16.105	27.115	10.563	1.00 36.61	c
ATOM	229	CD	ARG	Α	44	14.638	26.534	10.809	1.00 39.09	Č
ATOM ·	230	NE	ARG	Α	44	14.350	25.140	10.395	1.00 41.98	N
MOTA	231	CZ	ARG		44	14.179	24.099	11.246	1.00 43.25	С
MOTA	232	NH1			44	14.332	24.244	12.561	1.00 40.76	N
ATOM	233		ARG		44	13.864	22.892	10.777	1.00 44.70	N
ATOM	234	N	LEU		45	19.878	25.118	8.428	1.00 31.29	N
MOTA	235	CA	LEU		45	20.544	24.560	7.294	1.00 30.82	С
MOTA	236	C	LEU		45	20.744	23.083	7.470	1.00 31.52	С
MOTA	237	0	LEU		45	20.690	22.550	8.597	1.00 31.99	0
MOTA MOTA	238 239	CB	LEU		45	21.909	25.221	7.134	1.00 29.63	С
MOTA	240	CG CD1	LEU		45	21.873	26.697	6.813	1.00 31.00	· C
ATOM	241		LEU LEU		45 45	23.279	27.338	7.030	1.00 31.79	C
MOTA	242	N	SER		46	21.403	26.918	5.378	1.00 31.14	C
ATOM	243	CA	SER		46	21.004 21.345	22.437 21.057	6.338 6.327	1.00 31.72 1.00 32.17	. й
ATOM	244	C	SER		46	22.771	20.978	6.767		. с
ATOM	245	ō	SER		46	23.568	21.871	6.562	1.00 32.55 1.00 31.31	
ATOM	246	CB	SER		46	21.255	20.447	4.936	1.00 32.06	0
ATOM	247	OG	SER		46	21.909	19.187	4.931	1.00 31.15	0
ATOM	248	N	GLN		47	23.068	19.849	7.358	1.00 33.60	N
ATOM	249	CA	GLN		47	24.370	19.546	7.878	1.00 34.42	C
MOTA	250	С	GLN		47	25.385	19.453	6.754	1.00 34.74	· c
ATOM	251	0	GLN		47	26.554	19.685	6.971	1.00 35.40	ō
ATOM	252	CB	GLN	A	47	24.232	18.194	8.593	1.00 35.09	Ċ
ATOM	253	CG	GLN	Α	47	25.465	17.417	8.733	1.00 36.19	С
ATOM	254	CD	GLN		47	25.670	16.422	7.678	1.00 36.93	С
MOTA	255	OE1			47	24.757	16.093	6.902	1.00 38.75	0
ATOM	256		GLN		47	26.894	15.903	7.630	1.00 40.53	N
ATOM	257	N	SER		48	24.933	19.095	5.556	1.00 34.63	N
ATOM	258	CA	SER		48	25.821	18.922	4.415	1.00 34.93	С
ATOM	259	C	SER		48	26.128	20.249	3.735	1.00 35.90	C
ATOM	260	0	SER		48	26.990	20.315	2.862	1.00 36.31	0
ATOM	261	CB	SER		48	25.182	17.991	3.381	1.00 34.59	С
ATOM	262	OG	SER		48 ·	23.912	18.483	2.955	1.00 33.48	0
ATOM	263	N	ASP		49	25.415	21.302	4.124	1.00 36.41	N
ATOM	264	CA	ASP	A	49	25.583	22.606	3.512	1.00 37.09	С

ATOM	265	C .	ASP	A	49	26.855	23.291	3.989	1.00 3	37.81	С	
ATOM	266		ASP	Α	49	27.020	23.523	5.182	1.00 3	36.99	0	
ATOM	267		ASP		49	24.383	23.451	3.877	1.00 3	37.42	С	
ATOM	268		ASP		49	24.323	24.733	3.117	1.00 3	38.29	С	
ATOM	269	OD1			49	25.383	25.351	2.849	1.00 3	37.80	0	
ATOM	270	OD2			49	23.223	25.191	2.760	1.00 4		0	
MOTA	271	N	PRO	A	50	27.740	23.649	3.056	1.00	38.39	N	
MOTA	272	CA	PRO	Α	50	29.005	24.291	3.409	1.00	38.24	С	
MOTA	273	С	PRO	A	50	28.802	25.502	4.285	1.00		C	
MOTA	274	0	PRO	A	50	29.671	25.797	5.088	1.00		0	
ATOM	275	CB	PRO	Α	50	29.577	24.738	2.051	1.00		C	
MOTA	276	CG	PRO	Α	50	28.978	23.915	1.070	1.00		C	
MOTA	277	CD	PRO		50	27.620	23.473	1.601	1.00		C	
MOTA	278	N	ARG		51	27.686	26.199	4.125	1.00		И	
ATOM	279	CA	ARG		51	27.448	27.403	4.912	1.00		C	
MOTA	280	С	ARG		51	27.332	27.077	6.391	1.00		C 0	
MOTA	281	0	ARG		51	27.668	27.908	7.259	1.00		C	
MOTA	282	CB	ARG		51	26.199	28.120	4.438	1.00		c	
ATOM	283	CG	ARG		51	26.372	28.781	3.067		41.10	C	
ATOM	284	CD	ARG		51	25.099	29.355	2.486		42.20 44.96	N	
ATOM	285	NE	ARG		51	24.111	28.314 28.551	2.192 2.043		46.68	C	
ATOM	286	CZ	ARG ARG		51 51	22.815 22.348	29.795	2.162		47.61	N	
ATOM ATOM	287 288		ARG		51	21.980	27.563	1.774		46.08	N	
ATOM	289	N	ALA		52	26.882	25.867	6.688		38.31	N	
ATOM	290	CA	ALA		52	26.729	25.498	8.082		38.63	С	
ATOM.	291	C	ALA		52	28.093	25.311	8.677	1.00	38.81	C	
ATOM	292	ō	ALA		52	28.341	25.682	9.816	1.00	39.03	0	
ATOM	293	CB	ALF		52	25.907	24.233	8.235	1.00	38.36	С	
ATOM	294	N	GLU	JΑ	53	28.988	24.733	7.899		39.48	N	
MOTA	295	CA	GLU	JA	53	30.316	24.484	8.388		40.51	C	
MOTA	296	С	GLU	JA		31.038	25.802	8.621		40.41	C	
MOTA	297	0	GL			31.740	25.954	9.618		39.82	0	
MOTA	298	CB	GL			31.093	23.614	7.436		40.70	C	
MOTA	299	CG		JA		32.129	22.790	8.171 8.633		44.79 48.98	c	
MOTA	300	CD		JA		31.596	21.435 21.329	9.017		51.56	. 0	
MOTA	301		GL			30.427 32.354	21.329	8.620		54.44	o	
MOTA	302 303	N	GLI	UA		30.851	26.752	7.713		40.45	N	
ATOM ATOM	303	CA		UA		31.465	28.060	7.853		41.40	C	
ATOM	305	C		UA		30.991	28.731	9.162		40.32	С	
ATOM	306	ŏ		UA		31.760	29.374	9.836	1.00	39.89	0	
ATOM	307	СВ		U A		31.119	28.974	6.679		42.12	С	
MOTA	308	CG		U A		31.697	28.557	5.333	1.00	47.25	С	
ATOM	309	CD		U A		30.953	29.191	4.129		53.54	C	
MOTA	310	OE:	l GL	U A	54	30.459	30.366	4.276		57.47	0	
MOTA	311	OE	2 GL	UA		30.882	28.527	3.036		53.82	0	
MOTA	312			U P		29.735	28.534	9.533		39.03	N	
MOTA	313			UP		29.223		10.687		37.80	C	
MOTA	· 314			U P		29.840		11.956		36.83	C	
MOTA	315			U F		30.293		12.795		35.66	0	
ATOM	316			U A		27.715		10.725 9.621		38.06 37.63	c	
MOTA	317			U I		27.072		9.449		39.63	c	
ATOM	318		1 LE			25.620 27.174		9.928		36.27	Č	
ATOM	319		2 LE	ic A		29.876		12.079		35.87	N	
ATOM	320 321			SE A		30.436		13.257		35.35	C	
MOTA MOTA	321			E A		31.916		13.410		35.82	Č	
ATOM	323			JE A		32.377		14.499		36.59	0	
MOTA	324			JE 2		30.281		13.139		34.84	C	
ATOM	325		1 II			28.790		13.132	1.00	34.00	С	
									•			

ATOM	326	CG2	ILE .	A !	56	31.022	24.535	14.280	1.00 34.89	c [.]
MOTA	327		ILE .		56	28.502	23.361	12.684	1.00 30.65	c
ATOM	328	N	GLU .		57	32.636	26.964	12.301	1.00 36.28	N
MOTA	329	CA	GLU		57	34.056	27.244	12.255	1.00 37.26	C
ATOM	330	С	GLU .		57	34.295	28.634	12.809	1.00 37.41	С
ATOM	331	0	GLU .		57	35.278	28.879	13.516	1.00 38.73	0
ATOM ATOM	332 333	CB CG	GLU		57 57	34.562	27.167	10.795	1.00 37.54	C
ATOM	334	CD	GLU GLU		5 <i>1</i> 57	36.035 36.948	27.462 26.668	10.572 11.493	1.00 39.41	C
ATOM	335		GLU		5 <i>7</i> 57	36.666	25.458	11.741	1.00 44.86 1.00 48.72	0.
MOTA	336	OE2			57	37.961	27.260	11.965	1.00 46.32	0
ATOM	337	N	ASN		58	33.386	29.537	12.485	1.00 36.64	N
MOTA	338	CA	ASN		58	33.456	30.907	12.926	1.00 36.26	Ĉ
MOTA	339	С	ASN		58	32.768	31.226	14.219	1.00 35.28	С
MOTA	340	0	ASN		58	32.569	32.376	14.531	1.00 33.45	0
ATOM	341	CB	ASN		58	32.798	31.758	11.898	1.00 36.88	C
MOTA	342	CG	ASN		58	33.763	32.461	11.107	1.00 39.77	C
MOTA MOTA	343 344		asn asn		58 58	34.140 34.241	31.983 33.617	10.018	1.00 41.34	0
ATOM	345	NDZ N	GLU		59	32.366	30.205	11.639 14.945	1.00 41.14 1.00 35.05	N N
ATOM	346	CA	GLU		59	31.706	30.415	16.226	1.00 35.00	C
ATOM	347	C	GLU		59	30.481	31.314	16.133	1.00 33.86	c
MOTA	348	0	GLU		59	30.293	32.238	16.904	1.00 33.16	Ö
MOTA	349	CB	GLU	A	59	32.729	30.855	17.244	1.00 34.95	C
MOTA	350	CG	GLU		59	33.708	29.700	17.423	1.00 37.79	С
MOTA	351	CD	GLU		59	34.652	29.820	18.586	1.00 39.57	С
ATOM	352	OE1			59	35.809	30.145	18.349	1.00 43.67	0
MOTA	353	OE2			59	34.254	29.545	19.723	1.00 45.29	0
MOTA MOTA	354 355	N CA	GLU GLU		60 60	29.644	30.995	15.157	1.00 32.92	N
MOTA	356	C	GLU		60	28.359 27.284	31.641 30.576	14.983 14.993	1.00 32.66 1.00 30.59	C C
ATOM	357	Ö	GLU		60	27.456	29.485	14.461	1.00 30.39	0
ATOM	358	СВ	GLU		60	28.312	32.400	13.685	1.00 33.20	Č
MOTA	359	CG	GLU		60	29.384	33.454	13.615	1.00 38.62	Ċ
MOTA	360	CD	GLU	A	60	28.955	34.617	12.762	1.00 45.73	C
MOTA	361	OE1			60	29.075	34.553	11.519	1.00 48.47	. 0
ATOM	362	OE2			60	28.466	35.587	13.367	1.00 53.89	0
ATOM	363	N	PRO		61	26.152	30.915	15.560	1.00 28.63	N
ATOM	364	CA	PRO		61	25.073	29.954	15.735	1.00 28.05	C
ATOM ATOM	365 366	С 0	PRO PRO		61 61	24.462 24.475	29.451 · 30.120	14.443	1.00 27.61	C
ATOM	367	CB	PRO		61	24.475	30.754	13.426 16.492	1.00 27.23 1.00 28.67	. 0
ATOM	368	CG	PRO		61	24.385	32.140	16.492	1.00 23.07	C C
ATOM	369	CD	PRO		61	25.811	32.253	16.038	1.00 27.71	Č
ATOM		N	VAL		62	23.936	28.237	14.475	1.00 27.43	N
ATOM		CA	VAL	Α	62	23.254	27.685	13.317	1.00 27.09	С
ATOM	372	С	VAL		62	22.372	26.569	13.802	1.00 27.40	·C
ATOM	373	0	VAL		62	22.707	25.893	14.780	1.00 27.79	0
ATOM	374	CB	VAL		62	24.219	27.181	12.270	1.00 27.04	C
MOTA MOTA			VAL		62	25.106	26.166	12.829	1.00 27.34	C
ATOM		N	VAL VAL		62 63	23.473	26.659	11.037	1.00 27.58	C
MOTA		CA	VAL		63	21.195 20.339	26.440 25.338	13.199 13.526	1.00 27.19 1.00 27.37	N C
ATOM		C	VAL		63	20.540	24.324	12.383	1.00 27.37	C
ATOM		ō	VAL		63	20.340	24.672	11.208	1.00 27.05	0
ATOM		СВ	VAL		63	18.857	25.737	13.611	1.00 27.47	Č
ATOM	382		. VAL		63	17.976	24.446	13.695	1.00 28.55	C
MOTA			VAL		63	18.616	26.603	14.793	1.00 25.77	С
MOTA		N	LEU		64	20.933	23.114	12.743	1.00 27.26	N
MOTA		CA	LEU		64	21.119	22.001	11.820	1.00 28.51	C
. ATOM	386	С	LEU	A	64	19.897	21.128	11.894	1.00 28.40	С

					. 00 00 60
ATOM	387 O LEU A 64	19.517			1.00 28.69
MOTA	388 CB LEU A 64	22.352			1.00 28.92
ATOM	389 CG LEU A 64	23.624			1.00 31.65
ATOM	390 CD1 LEU A 64	24.800	21.273		1.00 34.84
ATOM	391 CD2 LEU A 64	23.843	22.490		1.00 35.77
ATOM	392 N THR A 65	19,284	20.868		1.00 28.44
ATOM	393 CA THR A 65	18.003	20.164	10.721	1.00 29.54
ATOM	394 C THR A 65	18.054	18.659		1.00 29.40
ATOM	395 O THR A 65	17.046	17.985	10.799	1.00 29.20
ATOM	396 CB THR A 65	17.139	20.679	9.552	1.00 30.07
ATOM	397 OG1 THR A 65	17.879	20.569		1.00 30.75
	398 CG2 THR A 65	16.878	22.137	9.665	1.00 31.86
ATOM	399 N ASP A 66	19.183	18.150	10.059	1.00 29.30
ATOM		19.323	16.722	9.719	1.00 29.78
ATOM		20.573	15.970	10.196	1.00 29.12
ATOM		21.081	15.141	9.432	1.00 29.09
MOTA			16.582	8.195	1.00 29.41
MOTA	403 CB ASP A 66	19.301		7.525	1.00 32.36
MOTA	404 CG ASP A 66	20.274	17.507		1.00 32.30
MOTA	405 OD1 ASP A 66		18.319	8.230	1.00 34.87
'ATOM	406. OD2 ASP A 66		17.534	6.287	
MOTA	407 N THR A 67		16.254	11.404	1.00 28.05
MOTA	408 CA THR A 67		15.565	11.897	1.00 27.24
MOTA	409 C THR A 67		14.171	12.355	1.00 26.92
MOTA	410 O THR A 67		13.297	12.367	1.00 25.98
MOTA	411 CB THR A 67	22.856	16.258	13.134	1.00 27.78
ATOM	412 OG1 THR A 67	21.874	16.338	14.186	1.00 25.71
ATOM	413 CG2 THR A 67	23.268	17.664	12.820	1.00 29.22
ATOM	414 N ASN A 68		13.979	12.777	1.00 26.53
ATOM	415 CA ASN A 68		12.711	13.355	1.00 27.10
ATOM	416 C ASN A 68		12.499	14.647	1.00 26.46
ATOM	417 O ASN A 68		11.399	15.092	1.00 26.90
ATOM	418 CB ASN A 68		11.547	12.401	1.00 27.41
ATOM	419 CG ASN A 68		11.415	11.308	1.00 28.18
	420 OD1 ASN A 68		11.286	11.566	1.00 29.22
ATOM	420 ODI ASN A 6			10.077	1.00 29.40
MOTA	422 N LEU A 6			15.227	1.00 26.58
ATOM	_			16.427	1.00 26.67
ATOM				17.558	1.00 26.73
MOTA				18.166	1.00 27.74
ATOM	•			16.968	1.00 26.04
ATOM		•		18.157	1.00 26.23
MOTA	427 CG LEU A 6	- 04 000		17.894	1.00 27.92
MOTA	428 CD1 LEU A 6				1.00 24.74
ATOM		9 23.976			1.00 24.71
MOTA		0 .20.557			1.00 26.50
MOTA		0 19.882			1.00 26.71
MOTA		0 18.673			1.00 25.71
MOTA		0 17.650			1.00 25.35
MOTA		0 19.479			1.00 28.17
MOTA		0 20.71			
MOTA	_	0 18.51			
MOTA		18.83			
MOTA		17.79			1.00 29.60
MOTA		17.09			
MOTA		15.90			
ATOM	441 CB TYR A	11 18.32			
MOTA		71 17.34			
ATOM		71 16.13			
ATOM	444 CD2 TYR A	71 17.61			
ATOM		71 15.22			1.00 31.86
ATOM		71 16.73			
ATOM		71 15.55	6.558	3 13.755	1.00 31.10

ATOM	448	OH	TYR Z	A	71	14.698	5.530	13.342	1.00 39.44	Ö
ATOM	449	N	PRO I		72	17.807	8.317	18.108	1.00 30.56	N
ATOM	450	CA	PRO 2		72	17.150	7.336	18.991	1.00 30.85	C
ATOM	451	C	PRO 2		72	16.389	7.914	20.158	1.00 30.85	С
ATOM	452	0	PRO .		72	15.549	7.233	20.750	1.00 30.12	0
MOTA	453	CB	PRO		72	18.310	6.468	19.507	1.00 30.71	C
ATOM ATOM	454 455	CG CD	PRO .		72 72	19.420 19.268	6.692 8.158	18.515	1.00 31.79	C
ATOM	456	И	ALA .		73	16.650	9.166	18.096 20.508	1.00 30.88 1.00 31.72	C N
ATOM	457	CA	ALA		73 73	15.918	9.743	21.627	1.00 31.72	. C
ATOM	458	C	ALA		73	14.596	10.371	21.172	1.00 31.71	č
ATOM	459	ō	ALA		73	13.786	10.808	22.000	1.00 31.52	Ö
ATOM	460	СВ	ALA		73	16.762	10.742	22.340	1.00 32.17	Ċ
ATOM	461	N	LEU		7.4	14.345	10.408	19.868	1.00 31.19	N
ATOM	462	CA	LEU	Α	74	13.108	11.028	19.439	1.00 32.01	С
MOTA	463	С	LEU	A	74	11.856	10.343	19.965	1.00 32.30	С
MOTA	464	0	LEU	Α	74	10.807	10.914	19.963	1.00 31.90	0
MOTA	465	CB	LEU		74	13.050	11.191	17.931	1.00 31.25	С
ATOM	466	CG	LEU		74	14.140	12.103	17.400	1.00 34.53	С
ATOM	467		LEU		74	13.904	12.418	15.965	1.00 37:35	С
ATOM	468		LEU		74	14.264	13.436	18.200	1.00 34.44	С
ATOM	469	N	LYS		75 75	11.963	9.100	20.396	1.00 34.18	N
ATOM ATOM	470	CA	LYS		75 75	10.802	8.376	20.910	1.00 34.36	C
ATOM	471 472	C O	LYS LYS		75 75	10.618 9.575	8.616 8.304	22.403 22.945	1.00 35.18 1.00 35.70	C
ATOM	473	CB	LYS		75 75	10.950	6.876	20.631	1.00 33.70	0 C
ATOM	474	CG	LYS		75 ·	12.138	6.219	21.294	1.00 34.31	C
ATOM	475	CD	LYS		75 75	12.302	4.754	20.834	1.00 33.13	C
ATOM '	476	CE	LYS		75	13.796	4.304	20.744	1.00 29.70	Č
ATOM	477	NZ	LYS		75	14.460	4.158	22.026	1.00 28.79	N
ATOM	478	N	TRP		76	11.619	9.181	23.071	1.00 35.44	N
MOTA	479	CA	TRP		76	11.517	9.426	24.495	1.00 36.05	C
MOTA	480	С	TRP	A	76	10.307	10.264	24.893	1.00 37.47	С
MOTA	481	0	TRP	A	76	9.958	11.222	24.212	1.00 38.43	0
MOTA	482	CB	TRP		76	12.742	10.179	24.994	1.00 35.67	С
MOTA	483	CG	TRP		76	13.980	9.395	24.963	1.00 33.87	С
ATOM	484	CD1	TRP		76 .	14.136	8.116	24.520	1.00 32.29	С
ATOM	485	CD2			76	15.252	9.821	25.409	1.00 30.36	C
ATOM	486	NE1			76 .	15.440	7.723	24.673	1.00 30.42	N
ATOM	487	CE2			76	16.143	8.754	25.221	1.00 28.82	C
ATOM ATOM	488 489	CE3	TRP TRP		76 76	15.739	11.013	25.954 25.560	1.00 29.45	C
ATOM	490		TRP		76 76	17.471 17.056	8.833 11.091	26.291	1.00 30.56 1.00 29.56	C C
ATOM	491	CH2			76 76	17.030	10.017	26.092	1.00 29.30	c
ATOM	492	N	ASP		77	9.698	9.894	26.014	1.00 38.14	И
MOTA	493	CA	ASP		77	8.620	10.640	26.635	1.00 38.33	Č
ATOM	494	С	ASP		77	8.653	10.223	28.094	1.00 37.89	Č
ATOM	495	0	ASP		77	9.443	9.390	28.447	1.00 37.97	0
MOTA	496	CB	ASP	Α	77	7.283	10.353	25.974	1.00 38.71	. С
ATOM	497	CG	ASP	Α	77	6.882	8.904	26.049	1.00 39.50	С
MOTA	498		ASP		77	7.414	8.107	26.867	1.00 41.50	0
MOTA	499	OD2	ASP		77	6.006	8.472	25.299	1.00 41.98	0
ATOM	500	N	LEU		78	7.838	10.800	28.955	1.00 38.47	N
MOTA	501	CA	LEU		78	7.941	10.481	30.375	1.00 39.09	C
ATOM	502	C	LEU		78	7.734	9.002	30.662	1.00 39.89	C
MOTA	503	0	LEU		78 70	8.421	8.423	31.50,7	1.00 40.19	0
MOTA	504	CB	LEU		78 79	6.966	11.310	31.171	1.00 39.02	C
MOTA MOTA	505 506	CG CD1	LEU LEU		78 78	7.169 6.058	12.815	31.042	1.00 41.51	C
ATOM	507		LEU		78 78	8.522	13.567 13.216	31.764 31.618	1.00 42.72 1.00 42.31	C C
ATOM	508	N N	GLU		70 79	6.795	8.369	29.971	1.00 42.31	N
						5.,55	2.555		2.00 10.00	

ATOM	509	CA	GLU Z	A	79	6.557	6.948	30.212	1.00 41.43	, c
ATOM	510	C	GLU Z	A	79	7.794	6.086	29.909	1.00 40.84	C
MOTA	511	0	GLU 2	A	79	8.228	5.283	30.742	1.00 40.45	0
MOTA	512		GLU .		79	5.343	6.458	29.418	1.00 42.10	С
ATOM	513		GLU .		79	5.023	4.998	29.658	1.00 45.06	С
MOTA	514		GLU .		79	3.840	4.525	28.846	1.00 49.74	С
MOTA	515		GLU .		79	3.436	5.254	27.914	1.00 52.37	0
ATOM	516		GLU .		79	3.316	3.426	29.150	1.00 53.21	0
ATOM	517		TYR .		80	8.361	6.248	28.718	1.00 40.43	N
ATOM	518		TYR		80	9.559	5.495	28.362	1.00 40.14	С
ATOM	519		TYR		80 .	10.750	5.765	29.297	1.00 40.06	С
ATOM	520	0	TYR		80	11.485	4.844	29.664	1.00 39.72	o Ċ
ATOM	521	CB	TYR		80	9.946	5.832	26.946	1.00 39.96	0
ATOM	522	CG	TYR		80	11.193	5.147	26.420	1.00 39.51	C
ATOM	523				80	11.118	3.897	25.804	1.00 38.93	C
ATOM	524		TYR		80	12.433	5.768	26.490	1.00 36.89	C
ATOM	525		TYR		80	12.253	3.277	25.290	1.00 38.08	C
ATOM	526		TYR		80	13.562	5.154	25.993	1.00 38.15	C
MOTA	527	CZ	TYR		80	13.468	3.915	25.379	1.00 39.06	0
ATOM	528	OH.	TYR		80	14.604	3.319	24.863	1.00 38.99 1.00 39.68	И
ATOM	529	N	LEU		81	10.935	7017	29.688		C
ATOM	530	CA	LEU		81 81	12.061 11.858	7.362 6.806	30.565 31.978	1.00 40.01 1.00 39.86	C
MOTA	531	C					6.284	32.608	1.00 39.88	0
MOTA	532	O	LEU		81	12.792 12.314	8.889	30.604	1.00 39.47	C
ATOM	533 534	CB CG	LEU		81 81	12.765	9.532	29.287	1.00 39.36	c
ATOM	535		LEU		81	12.705	11.045	29.402	1.00 39.70	Č
ATOM	536		LEU		81	14.117	9.018	28.840	1.00 39.32	Č
ATOM	537	N N	GLN		82	10.645	6.932	32.482	1.00 39.32	N
ATOM ATOM	538	CA	GLN		82	10.346	6.415	33.804	1.00 40.30	Č
ATOM	539	CA	GLN		82	10.612	4.920	33.799	1.00 40.84	Ċ
ATOM	540	0	GLN		82	11.193	4.379	34.711	1.00 40.35	Ö
ATOM	541	СВ	GLN		82	8.900	6.688	34.164	1.00 41.40	. C
ATOM	542	CG	GLN		82	8.447	5.906	35.351	1.00 42.97	· c
ATOM	543	·CD	GLN		82	7.291	6.560	36.099	1.00 45.14	c
MOTA	544	OE1			82	6.662	7.502	35.616	1.00 44.10	Ō
ATOM	545		GLN		82	7.003	6.039	37.287	1.00 48.04	N
ATOM	546·		GLU		83	10.222	4.256	32.728	1.00 41.35	N
ATOM	547	CA	GLU		83	10.442	2.816	32.620	1.00 41.46	C
ATOM	548	C	GLU		83	11.926	2.444	32.465	1.00 40.81	С
MOTA	549	ō	GLU		83	12.350	1.407	32.958	1.00 41.13	0
ATOM	550	CB	GLU		83	9.610	2.243	31.472		С
MOTA	551	CG	GLU		83	9.609	0.728	31.366	1.00 44.77	С
MOTA	552	CD	GLU		83	8.878	0.018	32.514	1.00 49.16	С
MOTA	553		GLU		83	8.219	0.672	33.347	1.00 52.26	0
ATOM	554	OE2	GLU	Α	83	8.978	-1.220	32.606	1.00 53.23	0
ATOM	555	N	ASN	Α	84	12.743	3.298	31.854	1.00 39.81	N
MOTA	556	CA	ASN	Α	84 .	14.099	2.859	31.515	1.00 38.82	С
ATOM	557	С	ASN	Α	84	15.290	3.611	32.048	1.00 38.20	С
ATOM ·	558	0	ASN	A	84	16.402	3.117	31.919	1.00 36.98	0
MOTA	559	CB	ASN	Α	84	14.244	2.828	29.995	1.00 38.83	С
MOTA	560	CG	ASN	I A	84	13.301	1.865	29.349	1.00 38.45	С
MOTA	561		ASN			13.307	0.670	29.664	1.00 40.40	. 0
MOTA	562		ASN			12.480	2.365	28.441		N
MOTA	563	N	ILE	A	85	15.088	4.781	32.645		N
MOTA	564	CA	ILE			16.226	5.598	32.998		C
MOTA	565		ILE			16.929	5.280	34.307		C
MOTA	566		ILE			17.849	5.993	34.702		0
MOTA	567		ILE			15.827	7.056	32.932		C
MOTA	568		LILE			17.001	7.891	32.418		C
MOTA	569	CG2	2 ILE	A	85	15.291	7.544	34.266	1.00 39.22	С

ATOM	570	CD1	ILE A	85	16.618	9.347	32.148	1.00 40.41	С
MOTA	571	N	GLY A	86	16.513	4.227	34.993	1.00 38.59	N
MOTA	572	CA	GLY A	86	17.208	3.801	36.199	1.00 38.15	С
MOTA	573	C	GLY A	86	16.658	4.386	37.476	1.00 37.92	C
ATOM	574	0	GLY A	86	15.652	5.097	37.461	1.00 37.90	0
ATOM	575	N	ASN A	87	17.359	4.113	38.574	1.00 37.70	. N
ATOM	576 577	CA	ASN A	87 .	16.941	4.542	39.899	1.00 37.34	C
ATOM	577	C	ASN A	87	17.898	5.576	40.487	1.00 36.99	C
MOTA	578 579	O CB	ASN A	87 87	17.920 16.786	5.807 3.306	41.710 40.840	1.00 36.36 1.00 37.40	0
ATOM ATOM	580	N	GLY A	88	18.676	6.224	39.618	1.00 37.40	И
ATOM	581	CA	GLY A	88	19.593	7.272	40.056	1.00 37.00	C
ATOM	582	C	GLY A	88	18.855	8.506	40.541	1.00 36.61	Č
ATOM	583	Ö	GLY A	88	17.673	8.648	40.298	1.00 36.55	Ö
ATOM	584	N	ASP A	89	19.532	9.392	41.250	1.00 37.05	N
ATOM	585	CA	ASP A	89	18.882	10.640	41.687	1.00 37.92	С
ATOM	586	С	ASP A	89	18.812	11.654	40.548	1.00 37.52	С
ATOM	587	0	ASP A	89	19.724	11.713	39.730	1.00 37.73	0
MOTA	588	CB	ASP A	89	19.639	11.281	42.840	1.00 38.02	С
ATOM	589	CG	ASP A	89	19.342	10.639	44.165	1.00 40.19	C
MOTA	590		ASP A		18.398	9.813	44.252	1.00 44.15	0
MOTA	591		ASP A		20.002	10.918	45.186	1.00 42.25	0
ATOM	592	N	PHE A		17.734	12.438	40.491	1.00 37.19	N
ATOM	593	CA	PHE A		17.638	13.546	39.520	1.00 36.65	C
ATOM	594	C	PHE A		17.435	14.912	40.182	1.00 36.57	C
ATOM	595	0	PHE A		16.551	15.078	41.015	1.00 36.80	0
ATOM ATOM	596 597	CB CG	PHE A		16.512 16.793	13.310 12.200	38.516 37.551	1.00 35.79 1.00 35.34	C
ATOM	598		PHE A		16.627	10.870	37.931	1.00 33.34	C
ATOM	599		PHE A		17.235	12.472	36.275	1.00 34.10	Ċ
ATOM	600		PHE A		16.875	9.854	37.061	1.00 31.47	Č
ATOM	601		PHE A		17.488	11.452	35.404	1.00 35.32	Ċ
ATOM	602	CZ	PHE A		17.315	10.123	35.813	1.00 34.26	С
ATOM	603	N	SER A		18.257	15.886	39.803	1.00 36.85	N
MOTA	604	CA	SER A	91	18.077	17.264	40.278	1.00 37.16	С
MOTA	605	С	SER A	91	16.856	17.884	39.612	1.00 37.28	. C
ATOM	606	0	SER A	91	16.761	17.912	38.392	1.00 36.72	0
MOTA	607	CB	SER A		19.278	18.146	39.971	1.00 36.75	С
MOTA	608	OG	SER A		20.470	17.600	40.456	1.00 35.79	0
MOTA	609	N	VAL A		15.938	18.374	40.434	1.00 37.83	N
ATOM	610	CA	VAL A		14.740	19.022	39.963	1.00 38.40	C
ATOM	611	C	VAL 7		14.549	20.334	40.690	1.00 39.41	C
MOTA MOTA	612 613	O CB	VAL A		14.465 13.507	20.394 18.227	41.941 40.298	1.00 39.08 1.00 38.96	0 C
ATOM	614		VAL A		12.270	19.005	39.893	1.00 38.57	C
ATOM	615		VAL A		13.556	16.837	39.651	1.00 39.45	Č
ATOM	616	N	TYR A		14.426	21.386	39.895	1.00 39.95	N
MOTA	617	CA	TYR A		14.214	22.701	40.419	1.00 40.34	C
MOTA	618	C	TYR A		12.756	22.950	40.459	1.00 40.76	C
ATOM	619	0	TYR A		11.999	22.493	39.583	1.00 40.39	0
MOTA	620	CB	TYR A	A 93	14.897	23.729	39.529	1.00 40.89	С
MOTA	621	CG	TYR A	A 93	16.369	23.580	39.627	1.00 40.80	С
ATOM	622		L TYR A		17.067	24.135	40.681	1.00 40.79	С
ATOM	623		2 TYR A		17.042	22.801	38.743	1.00 41.05	С
ATOM	624		L TYR A		18.395	23.953	40.802	1.00 41.05	C
ATOM	625	CE			18.363	22.629	38.852	1.00 42.75	C
MOTA	626	CZ	TYR A		19.037	23.204	39.881	1.00 42.45	C
MOTA	627	OH	TYR A		20.372	22.965	39.971		0
MOTA	628	N	SER A		12.385	23.699	41.482	1.00 41.70	N
MOTA	629	CA C	SER A		11.014	24.053	41.743		C
ATOM	630	Ċ	SER A	A 94	10.965	25.565	41.855	1.00 43.09	C

MOTA	631	0	SER .	A	94		11.851	26.181	42.441	1.00 43.63	. 0
ATOM	632	CB	SER .	A	94		10.570	23.415	43.051	1.00 42.76	· C
ATOM	633	OG	SER .	Α	94		9.258	23.841	43.395	1.00 45.05	Ō
ATOM	634	N	ALA	Α	95		9.929	26.171	41.308	1.00 43.42	N
MOTA	635		ALA		95		9.839	27.607	41.323	1.00 43.49	C
ATOM	636	С	ALA		95		8.416	28.083	41.281	1.00 43.87	č
MOTA	637		ALA		95		7.520	27.416	40.789	1.00 43.95	Õ
ATOM	638	СВ	ALA		95		10.572	28.164	40.145	1.00 43.70	Č
ATOM	639	N	SER		96		8.219	29.287	41.770	1.00 44.66	Ŋ
ATOM	640	CA	SER		96		6.901	29.866	41.757	1.00 45.08	C
ATOM	641	C	SER		96		6.767	30.914	40.668	1.00 44.27	c
ATOM	642	Ö	SER		96		5.783	31.636	40.637	1.00 44.27	0
ATOM	643	СВ	SER		96		6.604	30.510	43.095	1.00 45.20	C
ATOM	644	OG	SER				5.384	31.199	42.973		
ATOM	645	N	THR		97		7.776	31.133		1.00 47.96	0
ATOM	646	CA							39.819	1.00 42.95	И
	647		THR		97		7.738	31.962	38.688	1.00 42.08	C
ATOM		C	THR		97		8.103	31.184	37.461	1.00 40.94	C
ATOM	648	0	THR		97		8.604	30.095	37.584	1.00 40.73	0
ATOM	649	CB	THR		97		8.779	33.088	38.826	1.00 42.48	
ATOM	650	OG1			97		8.964	33.707	37.546	1.00 43.60	0
ATOM	651	CG2	THR		97		10.209	32.544	39.156	1.00 42.12	C
ATOM	652	N	HIS		98		7.904	31.734	36.275	1.00 40.18	N
ATOM	653	CA	HIS		98	•	8.319	31.012	35.074	1.00 40.09	С
ATOM	654	С	HIS		98		9.840	31.036	34.883	1.00 39.78	С
ATOM	655	0	HIS		98	-	10.376	30.277	34.078	1.00 38.48	0
ATOM	656	CB	HIS			•	7.660		33.824	1.00 40.00	С
MOTA	657	CG	HIS		98		7.947	33.028	33.582	1.00 40.56	С
ATOM	658		HIS		98		7.297	34.041	34.259	1.00 40.13	N
MOTA	659		HIS		98		8.805	33.640	32.729	1.00 42.26	С
ATOM	660		HIS		98		7.741	35.212	33.841	1.00 37.08	C
ATOM	661	NE2	HIS	A	98		8.661	35.002	32.915	1.00 39.74	N
ATOM	662	N	LYS		99		10.526	31.883	35.652	1.00 39.73	N
ATOM	663	CA	LYS	A	99		11.948	32.082	35.476	1.00 40.45	С
MOŢA	664	C	LYS	Α	99		12.861	31.221	36.332	1.00 40.34	С
ATOM	665	0	LYS	Α	99		12.904	31.376	37.554	1.00 41.93	0
MOTA	666	CB	LYS	Α	99		12.279	33.535	35.730	1.00 40.89	С
ATOM	667	CG	LYS	A	99		11.819	34.443	34.624	1.00 43.12	
MOTA	668	CD	LYS	Α	99		12.466	35.806	34.753	1.00 46.04	С
ATOM	669	CE	LYS	Α	99		11.733	36.727	.35.711	1.00 48.26	
ATOM	670	NZ	LYS	A	99		10.662	37.495	35.003	1.00 49.55	
ATOM	671	N	PHE	A	100		13.622	30.335	35.700	1.00 39.70	. N
ATOM	672	CA	PHE	Α	100		14.554	29.487		1.00 39.48	С
ATOM	673	С	PHE	A	100		16.001	30.011	36.390	1.00 39.52	
ATOM	674	0	PHE	Α	100		16.874	29.435	35.718	1.00 38.87	
ATOM	675	CB			100		14.485	28.056	35.939	1.00 39.33	
MOTA	676	CG			100		13.266	27.328	36.377	1.00 38.47	
MOTA	677	CD1	PHE				12.059	27.519	35.725	1.00 36.20	
ATOM	678		PHE				13.327	26.441	37.443	1.00 37.31	
MOTA	679		PHE				10.960	26.846	36.125	1.00 36.52	
ATOM	680				100.		12.212	25.751	37.849	1.00 36.40	
ATOM	681	CZ			100		11.037	25.946	37.206	1.00 36.52	
ATOM	682	N			101		16.244	31.130	37.066	1.00 39.53	
ATOM	683	CA			101		17.592	31.667	37.170	1.00 39.36	
ATOM	684	C			101		18.548	30.642	37.787	1.00 39.88	
ATOM	685	Ö			101		18.345	30.152	38.899	1.00 39.47	
ATOM	686	СВ			101		17.574	32.912	38.036	1.00 39.47	
MOTA	687	CG			101		18.828	33.777	38.071	1.00 39.37	
ATOM	688		LEU				19.258	34.290	36.693	1.00 39.44	
ATOM	689		LEU				18.546	34.290	39.008	1.00 37.36	
ATOM	690	N			101		19.578				
ATOM	691	CA			102		20.623	30.297 29.415	37.032 37.507	1.00 41.10 1.00 41.59	
HIOH	031	O.A.	711	- ~	102		20.023	49.413	37.307	1.00 41.59	C

D M	600	_	mvn	70	100		20 007	20 611	1 00	40.00		~
TOM	692 693	С 0	TYR TYR			21.439 21.778	30.097 31.296	38.611 38.500		42.23 42.28		C
TOM	694	ÇB	TYR			21.778	29.048	36.370		42.28		0 C
TOM	695	CG	TYR			22.706	28.209	36.894		43.02		C
TOM	696		TYR			22.507	26.864	37.200		42.85		C
TOM	697					23.941	28.761	37.150		43.85		C
TOM	698					23.504	26.110	37.725		45.04		c
TOM	699	CE2	TYR			24.942	28.005	37.696		46.05		C
TOM	700	CZ	TYR			24.725	26.681	37.984		46.73		C
TOM	701	OH	TYR			25.752	25.915	38.544		52.49		0
MOT	702	N	TYR			21.759	29.340	39.657		42.12		N
TOM	703	CA	TYR	A	103	22.665	29.832	40.690	1.00	42.58		С
MOT	704	С	TYR	Α	103	23.632	28.750	41.207	1.00	41.98		С
MOT	705	0	TYR	Α	103	23.333	27.560	41.237		42.05		0
MOT	706	CB			103	21.901	30.435	41.843		43.03		C
TOM	707	CG			103	20.964	29.493	42.477		44.79		С
MOT	708	CD1				19.691	29.333	41.971		47.69		C
TOM	709	CD2				21.338	28.769	43.590		49.51		С
TOM	710	CE1	TYR			18.798	28.456	42.544		50.63		С
TOM	711	CE2			103	20.449	27.890	44.202		52.43	•	С
TOM	712	CZ			103	19.181	27.736	43.658		52.68		C
TOM TOM	713	И			103	18.297 24.809	26.875	44.234		56.40		0
TOM	714 715	CA			104 104	25.844	29.190 28.288	41.603 42.026		41.00 40.33		И С
TOM	716	C			104	25.842	28.250	43.530		39.98		C
TOM	717	Ö			104	26.177	29.224	44.219		38.58		o
TOM	718	СВ			104	.27.169	28.768	41.492		40.13	•	c
TOM	719	CG			104	28.310	27.929	41.958		42.26		Ċ
TOM	720		ASP			28.117	27.151	42.942		44.33		ō
MOT	721		ASP			29.429	27.989	41.393		42.30		Õ
TOM.	722	N			105	25.425	27.110	44.041		40.20		N
MOT	723	CA	GLU	Α	105	25.294	26.950	45.472	1.00	40.26		C
TOM	724	С	GLU	Α	105	26.605	27.213	46.228	1.00	39.92		C
TOM	725	0	GLU	Α	. 105	26.577	27.824	47.293	1.00	40.11		0
MOT	726	CB			. 105	24.747	25.570	45.744		40.54		С
MOT	727	CG			. 105	23.245	25.502	45.533		42.55		. C
TOM	728	CD			. 105	22.709	24.086	45.506		44.11		С
TOM	729	OE1			105	23.178	23.251	46.323		46.78		0
TOM	730	OE2			105	21.801	23.815	44.684		42.74		0
TOM	731 732	N CA			. 106 . 106	27.748	26.819	45.661		39.52		N
TOM TOM	733				106	29.041 29.370	26.991 28.419	46.336 46.623		39.53		C
TOM	734	С 0			106	30.199	28.697	47.471		39.68 40.24		С 0
TOM	735	СВ			106	30.221	26.479	45.504		39.89		c
TOM	736	CG			106	30.257	24.976	45.143		40.25		C
TOM	737	N			107	28.747	29.333	45.894		40.07		N
TOM	738	CA			107	29.043	30.740	46.031		39.35		C
TOM	739	C			107	28.061	31.421	46.937		39.82		
MOT	740	0			107	28.208	32.586	47.188		39.28		CO
TOM	741	CB			107	29.050	31.410	44.645	1.00	39.29		С
MOT	742	CG	LYS	P	107	30.329	31.155	43.827	1.00	37.47		С
TOM	743	CD			107	30.286	31.702	42.406	1.00	34.55		С
TOM	744	CE			107	31.606	31.470	41.651	1.00	33.57		C
MOT	745	ΝZ			107	31.607	31.880	40.178		30.95		N
TOM	746	N			108	27.071	30.707	47.458		41.78		N
TOM	747	CA			108	26.079	31.341	48.341		43.69		C
TOM	748	С			108	26.621	31.950	49.646		44.68		С
TOM	749	0			108	26.154	33.004	50.061		44.99		0
TOM	750 751	CB			108	24.923	30.396	48.594		44.05		С
TOM TOM	751 752	CG SD			108	24.195	30.105	47.282		46.49		C
IOM	152	จบ	ME.I	. #	108	22.723	29.125	47.315	1.00	51.54		S

MOTA	753 CE MET A 108	21.653 30.080 48.484 1.00 51.43
ATOM	754 N ALA A 109	27.630 31.341 50.254 1.00 46.34
ATOM	755 CA ALA A 109	28.211 31.855 51.510 1.00 47.87
ATOM	756 C ALA A 109	28.697 33.308 51.406 1.00 49.27
	757 O ALA A 109	28.533 34.114 52.323 1.00 49.44
MOTA		29.355 30.958 51.960 1.00 47.63
MOTA	758 CB ALA A 109	29.276 33.651 50.269 1.00 50.88
ATOM	759 N ASN A 110	
ATOM	760 CA ASN A 110	
MOTA	761 C ASN A 110	
ATOM	762 O ASN A 110	29.038 37.252 49.562 1.00 51.14
ATOM	763 CB ASN A 110	30.876 34.939 48.994 1.00 52.43
MOTA	764 CG ASN A 110	32.077 34.080 49.433 1.00 54.41
ATOM	765 OD1 ASN A 110	32.460 34.050 50.624 1.00 54.72
MOTA	766 ND2 ASN A 110	32.663 33.373 48.478 1.00 56.75
ATOM	767 N PHE A 111	27.484 35.651 49.632 1.00 52.59
ATOM	768 CA PHE A 111	26.404 36.598 49.409 1.00 53.32
ATOM	769 C PHE A 111	25.202 36.180 50.261 1.00 54.75
ATOM	770 O PHE A 111	24.149 35.801 49.749 1.00 54.37
ATOM	771 CB PHE A 111	26.053 36.693 47.923 1.00 52.83
MOTA	772 CG PHE A 111	27.058 37.461 47.107 1.00 50.42
	773 CD1 PHE A 111	28.283 36.907 46.791 1.00 49.93
ATOM		26.781 38.729 46.658 1.00 48.60
ATOM		29.205 37.609 46.044 1.00 49.18
ATOM	775 CE1 PHE A 111	
MOTA	776 CE2 PHE A 111	2.1.12
MOTA	777 CZ PHE A 111	
MOTA	778 N GLN A 112	
ATOM	779 CA GLN A 112	24.353 35.855 52.536 1.00 58.14
MOTA	780 C GLN A 112	22.970 36.399 52.192 1.00 58.29
ATOM	781 O GLN A 112	21.972 35.742 52.468 1.00 58.53
MOTA	782 CB GLN A 112	24.730 36.282 53.961 1.00 58.65
MOTA	783 CG GLN A 112	26.100 35.815 54.441 1.00 61.33
ATOM	784 CD GLN A 112	26.213 34.307 54.467 1.00 64.34
ATOM	785 OE1 GLN A 112	25.483 33.622 53.750 1.00 66.46
ATOM	786 NE2 GLN A 112	27.133 33.784 55.281 1.00 66.00
ATOM	787 N ASN A 113	22.919 37.581 51.580 1.00 58.45
ATOM	788 CA ASN A 113	21.653 38.222 51.240 1.00 58.79
ATOM	789 C ASN A 113	21.000 37.740 49.936 1.00 58.82
ATOM	790 O ASN A 113	19.971 38.284 49.536 1.00 59.69
ATOM	791 CB ASN A 113	21.813 39.759 51.171 1.00 58.81
ATOM	792 CG ASN A 113	22.160 40.387 52.525 1.00 59.17
ATOM	793 OD1 ASN A 113	21.863 39.824 53.593 1.00 57.49
ATOM	794 ND2 ASN A 113	22.786 41.567 52.482 1.00 58.34
	795 N PHE A 114	21.570 36.760 49.245 1.00 58.33
ATOM	796 CA PHE A 114	20.930 36.306 48.015 1.00 57.84
ATOM	•	19.922 35.220 48.334 1.00 57.57
ATOM	797 C PHE A 114	20.264 34.208 48.953 1.00 57.24
MOTA	798 O PHE A 114	- -
MOTA	799 CB PHE A 114	
MOTA	800 CG PHE A 114	
MOTA	801 CD1 PHE A 114	20.642 35.897 44.867 1.00 58.11
MOTA	802 CD2 PHE A 114	21.300 33.744 45.674 1.00 58.56
MOTA	803 CE1 PHE A 114	20.028 35.312 43.781 1.00 58.29
MOTA	804 CE2 PHE A 114	20.687 33.149 44.580 1.00 59.09
MOTA	805 CZ PHE A 114	20.050 33.937 43.630 1.00 58.80
ATOM	806 N LYS A 115	18.686 35.429 47.899 1.00 57.18
ATOM	807 CA LYS A 115	17.604 34.511 48.204 1.00 57.19
ATOM	808 C LYS A 115	17.037 33.942 46.903 1.00 57.17
MOTA	809 O LYS A 115	16.268 34.598 46.193 1.00 57.12
ATOM	810 CB LYS A 115	16.524 35.234 49.016 1.00 57.33
ATOM	811 N PRO A 116	17.384 32.699 46.610 1.00 56.97
ATOM	812 CA PRO A 116	17.042 32.097 45.319 1.00 57.01
ATOM	813 C PRO A 116.	15.554 31.979 45.151 1.00 56.69
AIOM		

MOTA	814	0	PRO A	116	14.864	31.676	46.103	1.00 57.	03	0
MOTA	815	CB	PRO A	116	17.672	30.701	45.378	1.00 57.	15	С
ATOM	816	CG	PRO A		18.474	30.658	46.662	1.00 57.	53	C
ATOM	817	CD	PRO A		18.045	31.763	47.522	1.00 57.		С
ATOM	818	N	ARG A		15.073	32.212	43.945	1.00 56.		Ŋ
ATOM	819	CA	ARG A		13.663	32.087	43.656	1.00 56.		С
ATOM	820	C	ARG A		13.335	30.639	43.332	1.00 56.		C
MOTA	821	0	ARG A		12.160	30.272	43.279	1.00 56.		0
MOTA MOTA	822 823	CB	ARG A SER A		13.280	32.971	42.508	1.00 56.		C
ATOM	824	N CA	SER A		14.350 14.083	29.810 28.393	43.110 42.878	1.00 55. 1.00 55.		И С
ATOM	825	C	SER A		14.003	27.511	43.809	1.00 55.		C
ATOM	826	Ö	SER A		16.022	27.895	44.174	1.00 54.		0
ATOM	827	СВ	SER A		14.322	28.029	41.415	1.00 54.		C
ATOM	828	OG	SER A		15.672	28.196	41.087	1.00 55.		Ö
ATOM	829	N ·	ASN A		14.381	26.362	44.211	1.00 53.		Ŋ
ATOM	830	CA	ASN A		15.089	25.412	45.060	1.00 53.		C
ATOM	831	С	ASN A		15.307	24.118	44.326	1.00 51.		С
MOTA	832	0	ASN A	119	14.472	23.705	43.552	1.00 51.	. 23	0
ATOM	833	CB	ASN A	119	14.277	25.063	46.311	1.00 54.	. 32	С
MOTA	834	CG	ASN A		13.711	26.272	46.994	1.00 57.		C
MOTA	835		ASN A		14.448	27.099	47.563	1.00 60.	. 84	0
MOTA	836		ASN A		12.384	26.384	46.964	1.00 61.		N
ATOM	837	N	ARG A		16.418	23.470	44.621	1.00 50.		N
ATOM	838	CA	ARG A		16.772	22.182	44.049	1.00 49.		C
ATOM	839	C	ARG A		16.388	21.062	44.999	1.00 49.		C
ATOM ATOM	840	O ·	ARG A		16.620	21.150	46.206		.40	0
ATOM	841 842	CB CG	ARG A		18.283 18.799	22.133 20.901	43.843 43.144	1.00 49		C
ATOM	843	CD	ARG A		20.318	20.812	43.144	1.00 47		C
ATOM	844	NE	ARG A		20.972	21.240	44.301	1.00 43		N
ATOM	845	CZ	ARG A		21.316	20.432	45.314	1.00 43		. C
ATOM	846		ARG A		21.053		45.277	1.00 40		N
ATOM	847		ARG A		21.921	20.942	46.379	1.00 41		N
ATOM	848	N	GLU A		15.801	20.010	44.451	1.00 49		N
ATOM	849	CA	GLU A		15.435	18.830	45.206	1.00 48		С
ATOM	850	С	GLU A	121	15.905	17.609	44.411	1.00 47	.95	C.
MOTA	851	0	GLU A	121	15.793	17.564	43.192	1.00 48	.02	. 0
MOTA	852	CB	GLU A		13.922	18.782	45.461		.38	С
ATOM	853	CG	GLU A		13.444	17.500	46.141		.77	С
ATOM	854	CD	GLU A		12.185	17.695	46.961	1.00 54		C
ATOM	855		GLU A		12.312	18.258	48.073	1.00 58		0
MOTA	856		GLU A		11.087	17.284	46.512	1.00 55		0
ATOM ATOM	857 858	N CA	GLU A		16.455	16.622	45.104 44.463	1.00 47		N
ATOM	859	CA	GLU A GLU A		16.938 15.848	15.423 14.400	44.463	1.00 46 1.00 45		C C
MOTA	860	ŏ	GLU A		15.313	14.220	45.666	1.00 45		0
ATOM	861	CB	GLU A		18.200	14.940	45.158	1.00 45		C
ATOM	862	CG	GLU A		19.346	15.921	45.063	1.00 44		c
ATOM	863	CD	GLU A		19.789	16.154	43.623	1.00 45		Č
ATOM	864		GLU A		19.985	15.144	42.902	1.00 44		0
MOTA	865		GLU A		19.925	17.337	43.207	1.00 42		0
MOTA	866	N	MET A		15.481	13,751	43.503	1.00 44		N
MOTA	867	CA	MET A		14.462	12.731	43.589			С
MOTA	868	С	MET A		14.657	11.712	42.503	1.00 43		С
ATOM	869	0	MET A		15.495	11.891	41.613	1.00 43		0
ATOM	870	CB	MET A		13.078	13.358	43.490	1.00 44		C
MOTA	871	CG	MET A		12.831	14.092	42.205	1.00 45		C
ATOM	872	SD	MET A		11.244	14.946	42.206	1.00 47		S
ATOM	873	CE N	MET A		11.648	16.411	43.089	1.00 47		C
ATOM	874	N	LYS Ą	144	13.880	10.638	42.603	1.00 42	. 3 /	N

				41 602 1 00 41 47
MOTA	875 CA LYS A 124	13.869	9.575	41.623 1.00 41.47
ATOM	876 C LYS A 124	12.958	10.026	40.469 1.00 40.66
ATOM	877 O LYS A 124	12.066	10.862	40.654 1.00 39.80
ATOM	878 CB LYS A 124	13.354	8.267	42.250 1.00 41.45
ATOM	879 CG LYS A 124	14.160	7.756	43.470 1.00 41.70
	880 CD LYS A 124	15.574	7.301	43.076 1.00 42.20
ATOM		16.451	6.989	44.273 · 1.00 41.37
ATOM		17.894	7.201	43.966 1.00 41.63
ATOM ·	882 NZ LYS A 124		9.460	39.284 1.00 39.69
MOTA	883 N PHE A 125	13.178		
ATOM	884 CA PHE A 125	12.463	9.889	
ATOM	885 C PHE A 125	10.981	9.729	38.257 1.00 38.85
ATOM	886 O PHE A 125	10.217	10.613	37.890 1.00 37.81
ATOM	887 CB PHE A 125	12.942	9.154	36.862 1.00 38.45
ATOM	888 CG PHE A 125	12.618	9.871	35.610 1.00 39.49
ATOM	889 CD1 PHE A 125	13.471	10.840	35.118 1.00 40.78
ATOM	890 CD2 PHE A 125	11.428	9.655	34.967 1.00 40.81
ATOM	891 CE1 PHE A 125	13.181	11.530	33.992 1.00 40.48
ATOM	892 CE2 PHE A 125	11.123	10.353	33.825 1.00 41.39
MOTA	893 CZ PHE A 125	12.008	11.300	33.335 1.00 41.11
	894 N HIS A 126	10.575	8.602	38.835 1.00 39.49
MOTA		9.161	8.342	39.044 1.00 39.91
ATOM		8.599	9.408	39.976 1.00 39.98
MOTA		7.455	9.821	39.830 1.00 39.26
MOTA	897 O HIS A 126		6.899	39.552 1.00 40.45
MOTA	898 CB HIS A 126	8.906		
MOTA	899 CG HIS A 126	9.034	6.727	
MOTA	900 ND1 HIS A 126	7.987	6.950	
MOTA	901 CD2 HIS A 126	10.092	6.367	41.801 1.00 41.92
MOTA	902 CE1 HIS A 126	8.403	6.759	43.140 1.00 43.22
MOTA	903 NE2 HIS A 126	9.676	6.405	43.108 1.00 42.45
MOTA	904 N GLU A 127	9.428	9.898	40.890 1.00 40.59
ATOM	905 CA GLU A 127	8.975	10.919	41.824 1.00 41.56
MOTA	906 C GLU A 127	8.749	12.213	41.062 1.00 41.66
ATOM	907 O GLU A 127	7.774	12.941	41.294 1.00 41.64
ATOM	908 CB GLU A 127	9.968	11.102	42.978 1.00 41.64
MOTA	909 CG GLU A 127	10.149	9.839	
ATOM	910 CD GLU A 127	11.116		
	911 OE1 GLU A 127	12.326	10.217	
MOTA	912 OE2 GLU A 127	10.649	9.938	
ATOM		9.636		
MOTA	•	9.504		
MOTA	914 CA PHE A 128	8.213		
ATOM	915 C PHE A 128		14.537	
MOTA.	916 O PHE A 128			
MOTA	917 CB PHE A 128	10.708	13.864	
MOTA	918 CG PHE A 128	10.470		
MOTA	919 CD1 PHE A 128	10.199		
· ATOM	920 CD2 PHE A 128	10.537		
MOTA	921 CE1 PHE A 128	9.980		
MOTA	922 CE2 PHE A 128	10.329	15.191	
MOTA	923 CZ PHE A 128	10.044	16.510	
ATOM	924 N VAL A 129	7.999	12.463	37.921 1.00 43.85
MOTA	925 CA VAL A 129	6.813	12.288	37.095 1.00 44.87
ATOM	926 C VAL A 129	5.536		3 37.932 1.00 46.07
ATOM	927 O VAL A 129	4.574		
	928 CB VAL A 129	6.798		
ATOM	929 CG1 VAL A 129	5.496		
MOTA	930 CG2 VAL A 129	8.030		
MOTA		5.553		
MOTA		4.415		
ATOM	932 CA GLU A 130			
MOTA	933 C GLU A 130	4.136		
MOTA	934 O GLU A 130	3.003		
MOTA	935 CB GLU A 130	4.654	11.07	9 41.296 1.00 49.63

ATOM	936	CG	GLU A	A	130	4.5	534	9.576	4:	1.062	1.00	50.81	С
MOTA	937	CD	GLU A			5.2	257	8.747		2.117	1.00	53.77	C
MOTA	938		GLU A				666	9.295	4:	3.204	1.00	55.27	0
MOTA	939		GLU A				518	7.543		1.856		54.73	0
ATOM	940	N	LYS A				L70	14.121		0.798		50.56	N
MOTA	941	CA	LYS A				010	15.547		1.082		51.84	C
MOTA	942	С	LYS Z				385	16.276		9.886	1.00	52.55	С
MOTA	943	0	LYS A				182	17.070		0.061	1.00	52.15	0
ATOM	944	CB	LYS A				340	16.209		1.438	1.00		C
MOTA	945	CG	LYS				554	16.568		2.907	1.00	53.75	C
ATOM	946	CD	LYS				249	17.944		3.054	1.00		C
ATOM	947	CE	LYS				379	18.168		4.448		58.66	C
ATOM ATOM	948 949	NZ N	LYS				247	19.628		4.725		59.31	N
ATOM	950	CA	LEU A				845 247	16.014 16.691		8.667 7.513		53.84 55.23	N
ATOM	951	C	LEU :				762	16.408		7.407		55.96	C
ATOM	952	Ö	LEU .				973	17.292		7.063		55.69	Ö
ATOM	953	CB	LEU				906	16.278		6.206		55.45	Č
ATOM	954	CG	LEU				301	16.811		5.966		56.60	Ċ
MOTA	955	CD1					785	16.291		4.646		57.60	Č
ATOM	956		LEU				303	18.327		5.966		57.89	Ċ
ATOM .	957	. N	GLN .				397	15.157		7.669		57.19	N
ATOM .	958	CA	GLN .				998	14.739		7.663		58.15	C
ATOM	959	С	GLN				172	15.450		8.751	1.00	58.99	С
MOTA	960	0	GLN	Α	133	-0.	915	15.950	3	8.470	1.00	58.73	0
ATOM	961	CB	GLN	A	133	0.	897	13.230	3	7.824	1.00	58.03	С
MOTA	962	N	ASP	Α	134	0.	678	15.510	3	9.981	1.00	60.11	N
MOTA	963	CA	ASP			-0.	081	16.145	4	1.063	1.00	61.49	C
ATOM	964	С	ASP	A	134	-0.		17.629	4	0.783		61.55	С
ATOM	965	0	ASP			-1.		18.149		1.104		61.55	0
ATOM	966	CB	ASP				621	15.985		2.417		61.99	. С
ATOM	967	CG	ÀSP			-0.		16.454		3.587		64.74	· c
ATOM	968		ASP				310	17.082		3.346		67.52	0
MOTA	969		ASP				022	16.237		4.791		69.05	0
MOTA	970	N	ILE				594	18.312		0.179		61.80	N
ATOM	971	CA	ILE				402	19.706		9.860		62.08	· C
MOTA	972	C	ILE				700	19.856		88.823		62.29	C
ATOM ATOM	973 974	O CB	ILE		135		639	20.620		39:013		61.91	0
ATOM	975		ILE				711 - 705	20.301 20.391		39.366 10.528	1.00	62.21	C
ATOM	976		ILE				478	21.670		88.783		62.19	C
ATOM	977		ILE				157	20.437		0.100		62.96	C
ATOM	978	N			136		593	19.112		37.733		62.99	Ŋ
MOTA	979	CA			136		585	19.184		36.674		63.71	C
ATOM	980	C			136		977	18.992		37.259		64.44	c
MOTA	981	0			136		844	19.856		37.123		64.73	ō
MOTA	982	CB			136		305	18.136		35.619		63.77	C
MOTA	983	N			137		170	17.871		37.948		65.12	N
MOTA	984	CA	GLN	A	137	· -4.	472	17.509		38.497		65.60	C
MOTA	985	С	GLN	A	137	-4.	989	18.540) 3	39.477		65.70	·c
MOTA	986	0	GLN	Α	137	-6.	175	18.871	. 3	39.447	1.00	66.17	0
MOTA	987	CB			137	-4.	421	16.117	7 3	39.161	1.00	65.72	C
ATOM	988	N			138		115	19.056		10.336		65.61	N
MOTA	989	CA			138		549	20.011		11.358		65.53	С
ATOM	990	C			138		578	21.441		10.823		64.96	С
ATOM	991	0			138		748	22.392		11.589		64.93	0
ATOM	992	CB			138		670	19.912		12.613		65.65	С
ATOM	993	CG			138		37.5	20.712		12.588		67.10	G
ATOM	994	CD			. 138		482	20.352		43.745		68.96	C
ATOM	995	NE			138		372	21.270		13.957		69.79	N
MOTA	996	CZ	ARG	A	138	0.	905	20.919	9 4	13.880	T.00	71.69	С

ATOM	997	NH1	ARG A	13	88	1.	238	19.674	· 4	3.569	1.00	72.88		N
ATOM	998	NH2	ARG A	13	88	1.	862	21.811	4	4.106	1.00	72.52		N
MOTA	999	N	GLY A	13	39	-4.	426	21.593	3	9.508	1.00	64.31		N
ATOM	1000	CA	GLY A	13	39	-4.	370	22.912	3	8.897	1.00	63.53		С
ATOM	1001	С	GLY F	13	39	-3.	401	23.874	3	9.578	1.00	62.69		С
ATOM	1002	0	GLY F	13	39	-3.	631	25.080	3	9.570	1.00	62.92		0
ATOM	1003	N	GLY A	1 14	10	-2.	312	23.357	4	0.148	1.00	61.58	•	N
ATOM	1004	CA	GLY A	1 14	40	-1.	345	24.183	4	0.861	1.00	60.52		С
ATOM	1005	C	GLY A	1 14	40	-0.	539	25.103	3	9.958	1.00	59.56		C
ATOM	1006	0	GLY A			-0.	449	24.867	3	8.748	1.00	59.45		0
ATOM	1007	N	GLU A	A 14	41	0.	041	26.159	4	0.530	1.00	58.05		N
ATOM	1008	CA	GLU A	A 14	41	0.	859	27.090) 3	9.748	1.00	56.92		C
MOTA	1009	С	GLU A	A 14	41	2.	366	26.751	. 3	9.832	1.00	54.97		С
ATOM	1010	0	GLU Z	A 1	41	3.	189	27.326	5 3	9.113	1.00	54.51		0
ATOM	1011	CB	GLU Z	A 1	41	0.	602	28.547	7 4	0.177	1.00	57.45		C
ATOM	1012	CG	GLU Z			-0.	707	29.171	1 3	39.680	1.00	59.67	•	С
MOTA	1013	CD	GLU Z	A 1	41	-0.	851	29.193	3 3	88.154	1.00	63.48		С
ATOM	1014	OE1	GLU Z			0.	179	29.107	7 3	37.436	1.00	65.30		0
ATOM	1015	OE2	GLU 2	A 1	41	-2.	007	29.298	3 3	37.664	1.00	66.13		0
ATOM	1016	N	GLU :			2.	720	25.814	4	10.708	1.00	52.62		N
ATOM	1017	CA	GLU	A 1	42	4.	106	25.398	3 4	10.862	1.00	50.91		С
ATOM	1018	С	GLU .				679	24.958	3 3	39.516	1.00	48.93		С
MOTA	1019	0	GLU .			3.	960	24.477		38.641	1.00	48.64		0
ATOM	1020	CB	GLU .			4.	225	24.263	3 4	11.886	1.00	51.00		С
MOTA	1021	CG	GLU				656	24.005		42.352	1.00	51.76		. C
MOTA	1022	CD	GLU			5.	.814	22.81	1 4	43.282	1.00	52.64		C
MOTA	1023		GLU				871	22.009		43.447	1.00	55.52		0
ATOM	1024	OE2					. 911	22.66	7 .	43.855	1.00	53.97		0
ATOM	1025	N.	ARG			5	.979	25.13	9 :	39.356	1.00	46.58		N
ATOM	1026	CA	ARG	A 1	43	6	. 652	24.75	1 :	38.133	1.00	45.12		С
MOTA	1027	С	ARG	A 1	.43	7	.900	23.96	0	38.425	1.00	43.39		С
ATOM	1028	0	ARG	A 1	.43	8	.616	24.24	2	39.387	1.00	43.58		0
MOTA	1029	CB	ARG	A 1	.43	7	.069	25.98	3	37.360	1.00	45.52		С
ATOM	1030	CG	ARG	A 1	.43	5	.943	26.74	7	36.729	1.00	45.38		C
MOTA	1031	CD	ARG	A 1	.43	6	.488	27.89	9	35.969	1.00	46.06		С
MOTA	1032	NE	ARG	A 1	L43	5	.473	28.64	9	35.252	1.00	45.33		N
ATOM	1033	CZ	ARG	A 1	143	5	.194	28.49	1	33.984	1.00	42.93		С
ATOM	1034	NH1	ARG	A 1	L43	5	.836	27.57	3	33.253	1.00	41.86		N
MOTA	1035	NH2	ARG	A 1	L43	4	.257	29.25	2	33.452	1.00	43.53		N
ATOM	1036	N	LEU	A 1	144	8	.182	22.99	1	37.578	1.00	41.08		N
ATOM	1037	CA	LEU	A 1	L44	9	.337	22.16	3	37.784	1.00	39.63		С
MOTA	1038	С	LEU	A 1	L44	10	.213	22.16	6 .	36.568		37.88		С
MOTA	1039	0	LEU	A 1	144	9	.734	22.24	9	35.444		36.26		0
MOTA	1040	CB	LEU	A 1	144	8	.889	20.72	:7	38.018	1.00	40.26		С
MOTA	1041	CG	TEU	A :	144	7	.974	20.52	9	39.223	1.00	41.73		С
MOTA	1042	CD1	LEU	A :	144	7	.639	19.03	86	39.392		42.57		С
MOTA	1043	CD2	LEU	A :	144	8	.585	21.10	2	40.503		41.42		С
ATOM	1044	N	TYR	A :	145	11	.507	22.03		36.800		36.36		N
MOTA	1045	CA	TYR	A :	145	12	.434	21.89	92	35.703		35.24		С
ATOM	1046	C	TYR	A :	145	13	.485	20.86	52	36.107	1.00	34.89		С
MOTA	1047	0	TYR	A :	145	14	.264	21.09	86	37.013	1.00	33.74		0
ATOM	1048	CB	TYR	A :	145	13	.071	23.24	13	35.352		35.01		С
ATOM	1049	CG	TYR	A	145	13	.524	23.40	80	33.901		32.68		С
MOTA	1050	CD:	l TYR	A	145	13	3.817	22.32	24	33.099		30.20		С
ATOM	1051	. CD	2 TYR	A	145	13	689	24.66	56	33.355		31.53		С
MOTA	1052	CE:	1 TYR	Α	145	14	.237			31.762		29.87		С
MOTA	1053	CE:	2 TYR	A	145	14	.110			32.031		29.82		С
MOTA	1054					14	1.373	23.76	65	31.228	1.0	30.06		С
MOTA	1055	он он				14	1.789			29.897		0 28.17		0
MOTA	1056	5 N	LEU	A	146	13	3.479			35.446		0 34.87		N
ATOM	1057	CA	LEU	A	146	14	1.511	18.70	03	35.690	1.0	0 35.40		С

ATOM	1058	С	LEU A 1	L46	15.753	18.977	34.864	1.00 35.24	С
MOTA	1059	0	LEU A		15.665	19.211	33.653	1.00 34.63	0
MOTA	1060	CB	LEU A		14.008	17.312	35.358	1.00 35.79	С
MOTA	1061	CG	LEU A		14.998	16.157	35.614	1.00 37.21	C
MOTA	1062		LEU A		14.221	14.918	35.969	1.00 36.28	C
MOTA	1063		LEU A :		15.907	15.872	34.399	1.00 38.78	С
MOTA	1064	N	GLN A		16.907	18.883	35.515	1.00 34.82	N
MOTA	1065	CA	GLN A		18.179	19.206	34.884	1.00 35.00	C
ATOM	1066	С	GLN A		19.222	18.341	35.525	1.00 34.90	С
ATOM	1067	0	GLN A		19.626	18.568	36.664	1.00 35.65	0
MOTA	1068	CB	GLN A		18.526	20.679	35.078	1.00 35.09	С
ATOM	1069	CG	GLN A		17.392	21.636	34.720	1.00 35.83	C
ATOM	1070	CD	GLN A		17.848	23.085	34.706	1.00 36.90	C
ATOM	1071	OE1			17.091	23.961	34.302	1.00 39.61	0
ATOM	1072	NE2			19.088	23.336	35.126	1.00 35.05	N
ATOM	1073	N	GLN A		19.673	17.358	34.773	1.00 35.00	N
ATOM	1074	CA	GLN A		20.492	16.300	35.294	1.00 34.89	C
ATOM	1075	C	GLN A		21.376	15.709 15.318	34.255	1.00 35.35	C
ATOM ATOM	1076 1077	O CB	GLN A GLN A		20.941		33.181	1.00 35.25	0
ATOM	1077	CG .	GLN A		19.580 20.335	15.186 13.914	35.791 36.269	1.00 35.27 1.00 35.11	C
ATOM	1079	CD	GLN A		21.317	14.230	37.389	1.00 33.11	c
ATOM	1080	OE1			20.998	15.033	38.277	1.00 34.12	0
ATOM	1081	NE2			22.521	13.652	37.324	1.00 33.10	N
ATOM	1082	N	THR A		22.631	15.641	34.600	1.00 36.56	N
ATOM	1083	CA	THR A		23.648	15.088	33.754	1.00 38.26	C
ATOM	1084	C	THR A		23.394	13.609	33.615	1.00 38.31	Ċ
ATOM	1085	Ö	THR A		23.068	12.956	34.597	1.00 38.70	Ö
ATOM	1086	СВ	THR A		24.992	15.362	34.463	1.00 38.76	c
ATOM	1087	OG1			25.290	16.747	34.277	1.00 41.68	ō
MOTA	1088	CG2			26.139	14.710	33.797	1.00 40.77	C
MOTA	1089	N	LEU A		23.516	13.087	32.399	1.00 38.77	N
MOTA	1090	CA	LEU A		23.373	11.664	32.149	1.00 39.27	С
MOTA	1091	С	LEU A		24.604	10.898	32.679	1.00 39.85	С
MOTA	1092	0	LEU A	150	25.733	11.207	32.321	1.00 39.99	0
MOTA	1093	CB	LEU A		23.220	11.402	30.660	1.00 39.15	. С
MOTA	1094	CG	LEU A		21.943	11.860	29.962	1.00 40.72	С
MOTA	1095		LEU A		22.058	11.673	28.459	1.00 41.91	С
MOTA	1096		LEU A		20.764	11.106	30.458	1.00 41.30	C
MOTA	1097	N	ASN A		24.392	9.898	33.526	1.00 40.26	N
ATOM	1098	CA	ASN A		25.510	9.124	34.062	1.00 40.90	С
MOTA	1099	C	ASN A		25.291	7.607	34.041	1.00 41.95	С
ATOM	1100	0	ASN A		24.327	7.098	33.441	1.00 41.72	0
ATOM	1101	CB	ASN A		25.778	9.575	35.489	1.00 40.77	C
MOTA	1102	CG	ASN A		24.564	9.439		1.00 39.85	. C
MOTA			ASN A		24.002	8.340	36.483	1.00 37.92	0
ATOM	1104		ASN A		24.107	10.558	36.897	1.00 36.89	N
ATOM	1105 1106	N	ASP A		26.176	6.894	34.735	1.00 42.89	N
ATOM ATOM	1107	CA	ASP A		26.175	5.431	34.756	1.00 43.75	C
ATOM	1107	C O	ASP A		24.950 24.787	4.768 3.581	35.272	1.00 43.37	C
ATOM	1103	СВ	ASP A		27.256	4.895	35.052 35.695	1.00 43.66 1.00 44.77	. 0 C
ATOM	1110	CG	ASP A		28.539	5.555	35.500	1.00 44.77	C
ATOM	1111		L ASP A		28.835	5.881	34.325	1.00 48.22	0
ATOM	1112		ASP A		29.291	5.826	36.437	1.00 57.47	0
ATOM	1113	N N	THR A		24.119	5.466	36.025	1.00 31.28	N
ATOM	1114	CA	THR A		22.983	4.783	36.631	1.00 43.41	C
ATOM	1115	C	THR A		21.820	4.605	35.676	1.00 42.99	c
ATOM	1116	Ö	THR A		20.866	3.945	36.012	1.00 43.44	ő
ATOM	1117	СВ	THR A		22.489	5.507	37.875	1.00 43.44	c
MOTA	1118	OG1	L THR A		21.749	6.678	37.499	1.00 46.09	Ō

ATOM	1119	CG2	THR A 15	3	23.651	6.008	38.725	1.00			С
MOTA	1120		VAL A 15		21.874	5.185	34.491	1.00			N
MOTA	1121		VAL A 15		20.757	5.015	33.572	1.00			C
MOTA	1122		VAL A 15		20.700	3.563	33.177	1.00			C
MOTA	1123		VAL A 15	-3	21.729	2.892	33.193	1.00			0
MOTA	1124		VAL A 15		20.889	5.875	32.300	1.00			C C
MOTA	1125		VAL A 15		20.857	7.347	32.660		43.04		C
MOTA	1126		VAL A 15		22.159	5.516	31.538		42.56	•	N
ATOM	1127	N	GLY A 15		19.502	3.097 1.725	32.814 32.411		42.11 41.52		C
ATOM	1128	CA	GLY A 15		19.261	1.725	30.992		41.85		C
ATOM	1129	C	GLY A 15		19.642	2.140	30.123		41.87		Ö
ATOM	1130	0	GLY A 15		19.977 19.512	0.012	30.750		41.36		N
ATOM	1131	N CA	ARG A 15		19.961	-0.623	29.511		40.88		C
ATOM	1132 1133	CA	ARG A 15		19.397	-0.005	28.247		40.03		Č
MOTA MOTA	1134	o	ARG A 15			0.304	27.339		40.36		ō
ATOM	1134	СВ	ARG A 15		19.670	-2.148	29.555		40.77		C
ATOM	1136	И	LYS A 15		18.090	0.146	28.181	•	39.16		N
MOTA	1137	CA	LYS A 15		17.503	0.697	26.990		38.81		С
MOTA	1138	C	LYS A 15		18.078	2.114					С
ATOM	1139	Ö	LYS A 15		18.363	2.464			37.97		0
ATOM	1140	СВ	LYS A 15		15.968	0.714	27.090		39.20		С
ATOM	1141	CG	LYS A 15		15.266	-0.575	26.642		36.80		С
ATOM	1142	N	ILE A 15		18.268	2.909	27.791		37.56		N
ATOM	1143	CA	ILE A 15		18.759	4.287	27.606		37.28		С
ATOM	1144	C	ILE A 15		20.180 .		27.126	1.00	37.22		С
ATOM	1145	Ō	ILE A 1		20.582	5.120	26.302	1.00	37.08		0
ATOM	1146	СВ	ILE A 1		18.692	5.101	28.882	1.00	36.72		C
MOTA	1147		ILE A 1			. 5.220	29.356	1.00	37.17		С
ATOM	1148		ILE A 1		19.254	6.465	28.646	1.00	36.48		С
ATOM	1149		ILE A 1		16.359	5.900	28.409	1.00	38.28		С
MOTA	1150	N	VAL A 1		20.934	3.335	27.655	1.00	36.85		N
ATOM	1151	CA	VAL A 1		22.319	3.177	27.284	1.00	37.05		С
ATOM	1152	С	VAL A 1		22.349	2.864	25.785	1.00	36.45		С
ATOM	1153	0	VAL A 1	59	23.165	3.410	25.057	1.00	35.81		0
MOTA	1154	CB	VAL A 1	59	22.988	2.042	28.096		37.36	•	С
ATOM	1155	CGI	L VAL A 1	59	24.248	1.567	27.427		38.43		C
MOTA	1156	CG2	VAL A 1		23.302	2.499	29.494		37.81		С
MOTA	1157		MET A 1		21.453	1.990	25.339		35.84		N
MOTA	1158				21.369	1.637	23.910		36.30		C
MOTA	1159		MET A 1		21.064	2.883	23.074		34.46		C
MOTA	1160				21.715	3.142			33.88		0
MOTA	1161		MET A 1		20.294	0.576			36.83		C
MOTA	1162		MET A 1		20.654	-0.763			39.89		c s
MOTA	1163		MET A 1		21.916	-1.579			46.87		C
MOTA	1164		MET A 1		21.005	-1.940			47.08 33.13		N
ATOM	1165		ASP A 1		20.078	3.648			32.80		C
ATOM	1166				19.732	4.901			31.75		C
ATOM	1167		ASP A 1		20.931 21.209	5.877 6.425			31.06	•	o
ATOM	1168				18.598	5.553			32.93		Č
MOTA	1169				17.278	4.822			33.90		C
ATOM	1170		ASP A I		17.148				28.71		o
MOTA	1171 1172		2 ASP A		16.301	5.064			38.17		ő
ATOM ATOM	1173		PHE A		21.646				31.05		N
ATOM	1174				22.763				30.52		C
ATOM	1175		PHE A		23.835				28.89		c
ATOM	1176		PHE A		24.477				0 29.43		Ö
ATOM	1177				23.311				0 30.80		C
ATOM	1178				24.493				0 31.81		С
ATOM	1179		1 PHE A		24.325		25.904		0 35.81		С
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	4400			_				_				
MCM.	1180		PHE			25.770	7.322	25.653		35.00		С
ATOM	1181		PHE			25.430	10.000	26.197		35.94		С
ATOM	1182	CE2	PHE			26.887	8.143	25.941		35.90		С
MOTA	1183	CZ	PHE			26.711	9.467	26.202		35.61		С
ATOM	1184	N	LEU			24.067	5.271	22.914		28.19		N
ATOM	1185	CA	LEU			25.103	4.728	22.065		28.08		С
ATOM	1186	C	LEU			24.735	4.923	20.590		27.13		С
ATOM	1187	0	LEU			25.603	4.973	19.751		26.83		0
ATOM	1188	CB	LEU			25.306	3.244	22.368		27.86		С
ATOM	1189	CG	LEU			26.137	2.987	23.604		28.73		С
MOTA	1190		LEU			26.180	1.512	23.849		29.77		С
ATOM	1191		LEU		_	27.559	3.522	23.464		29.70		С
ATOM	1192	N	GLY			23.448	4.998	20.303		26.50		N
ATOM ATOM	1193	CA	GLY			22.956	5.244	18.959	1.00	27.37	•	С
	1194	C	GLY			22.949	6.712	18.493		27.88		С
ATOM ATOM	1195	0	GLY			22.483	6.988	17.365		28.42		0
ATOM	1196	N Cr	PHE			23.420	7:635	19.344		26.36		N
ATOM	1197 1198	CA	PHE			23.530	9.011	18.958		26.57		С
ATOM		C	PHE			24.540	9.052	17.820		26.12		C
ATOM	1199 1200	0	PHE			25.381	8.202	17.756		24.23		0
ATOM	1200	CB CG	PHE			24.024	9.867	20.153		26.86		С
ATOM	1201		PHE PHE			22.979	10.070	21.252	1.00	27.80		C
ATOM .	1202		PHE			21.701	9.533	21.144	1.00	27.80		C
ATOM	1203		PHE			23.274	10.820	22.367	1.00	28.58		C
ATOM	1204		PHE			20.765	9.744	22.117		26.89		C
ATOM	1206	CZ	PHE			22.329	11.042	23.364		28.45		C
ATOM	1207	N	ASN			21.086	10.504	23.243	1.00	28.78		С
ATOM	1208	CA	ASN			24.496	10.077	16.963	1.00	26.15		N
ATOM	1209	CA	ASN			25.441	10.165	15.837		25.91		C
ATOM	1210	Ö	ASN			26.861 27.288	10.675	16.226	1.00	26.12		C
ATOM	1211	CB	ASN			24.834	11.793	15.894	1.00	25.48		0
ATOM	1212	CG	ASN			25.634	11.004 10.916	14.705	1.00	25.51 24.43		C
ATOM	1213		ASN			26.751	10.323	13.431 13.429				С
ATOM	1214		ASN			25.078	11.479	12.318		23.40 17.22		0
ATOM	1215	N	TRP			27.566	9.817	16.940		26.11		N
ATOM	1216	CA	TRP			28.907	10.080	17.401	1.00	26.58		N C
ATOM	1217	C	TRP			29.817	10.336	16.206		27.07		C
ATOM	1218	ŏ			167	30.737	11.139	16.252		26.92		o
MOTA	1219	СВ	TRP			29.389	8.860	18.249	1.00	26.02		c
MOTA	1220	CG			167	28.537	8.750	19.498		27.18		C
MOTA	1221	CD1	TRP			27.620	7.784	19.809		28.08		c
MOTA	1222		TRP			28.452	9.719	20.550		27.33		c
MOTA	1223		TRP			27.013	8.071	21.013		27.87	-	N
MOTA	1224		TRP			27.503	9.254	21.481		26.46		C
MOTA	1225		TRP			29.103	10.929	20.804		26.22		Ċ
MOTA	1226		TRP			27.180	9.951	22.622		28.27		Č
MOTF	1227		TRP			28.784	11.615	21.920		27.56		Ċ
MOTE	1228	CH2	TRP	Α	167	27.821	11.128	22.833		28.04		C
MOTE	1229	N			168	29.585	9.632	15.114		27.98		N
MOTE	1230	CA			168	30.430	9.833	13.959		28.32		C
MOTE	1231	С	ASN	Α	168	30.470	11.319	13.573		29.00		С
MOTE	1232	0			168	31.547	11.894	13.390		30.41		ō
MOTE	1233	CB	ASN	A	168	29.909	9.018	12.812		28.58		Č
MOTE	1234	CG			168	30.758	9.145	11.570		29.28		C
MOTA	1235		ASN	Α	168	31.899	8.739	11.579		30.27		ō
MOTA	1236	ND2	ASN			30.186	9.677	10.487		28.46		N
MOT	1237	N			169	29.301	11.942	13.462		27.93		N
MOT	1238	CA			169	29.228	13.343	13.074		27.25		C
MOT	1239	C			169	29.726	14.266	14.179		27.20		Ċ
MOT	1240	0	TRP	Α	169	30.444	15.224	13.925		26.30		0

ATOM	1241	СВ	TRP A	169	27.777	13.734	12.691	1.00 26.63	С
MOTA	1242	CG	TRP A	169	27.615	15.168	12.355	1.00 25.15	. C
ATOM	1243	CD1	TRP P	169	27.804	15.745	11.130	1.00 24.89	С
ATOM	1244	CD2	TRP F	169	27.261	16.229	13.237	1.00 23.66	С
ATOM	1245	NE1	TRP F	169	27.591	17.095	11.195	1.00 22.98	N
ATOM	1246	CE2	TRP A	169	27.257	17.427	12.476	1.00 25.81	С
ATOM	1247		TRP A		26.927	16.292	14.576	1.00 24.44	C.
ATOM	1248		TRP A		26.933	18.680	13.018	1.00 26.96	С
ATOM	1249	CZ3	TRP A		26.624	17.525	15.127	1.00 28.68	С
ATOM	. 1250	CH2	TRP A		26.611	18.710	14.336	1.00 28.73	С
ATOM	1251	N.		A 170	29.323	14.026	15.409	1.00 27.29	N
MOTA	1252	CA	ILE A	A 170	29.725	14.985	16.406	1.00 28.36	С
MOTA	1253	С		A 170	31.252	14.874	16.686	1.00 29.15	С
ATOM	1254	0		A 170	31.920		16.866	1.00 29.81	0
ATOM	1255	CB		A 170	28.814	14.947	17.672	1.00 28.10	C
ATOM	1256	CG1		A 170	28.882	16.277	18.386	1.00 26.98	Ć
ATOM	1257			A 170	29.198	13.838	18.593	1.00 27.15	С
ATOM	1258			A 170	27.855	16.400	19.530	1.00 28.88	С
ATOM	1259	Ń		A 171	31.809	13.679	16.653	1.00 29.35	N
ATOM	1260	CA		A 171	33.261	13.535		1.00 30.18	С
ATOM	1261	C		A 171	34.060	14.259	15.752	1.00 30.67	С
ATOM	1262	Õ		A 171	35.117	14.823	16.036	1.00 31.32	0
ATOM	1263	СВ		A 171	33.705	12.058	16.861	1.00 29.80	.C
MOTA	1264	CG		A 171	33.210	11.274	18.094	1.00 30.17	С
ATOM	1265			A 171	32.682	11.821	19.051	1.00 30.65	0
ATOM	1266			A 171	33.372	9.968	18.036	1.00 31.44	N
ATOM	1267	N		A 172	33.591	14.231	14.509	1.00 30.94	N
ATOM	1268	CA		A 172	34.297	14.960	13.461	1.00 32.29	С
ATOM	1269	С		A 172	34.211	16.473	13.755	1.00 31.79	С
ATOM	1270	Ó		A 172	35.128	17.234	13.482	1.00 32.06	0
ATOM	1271	СВ		A 172	33.754	14.646	12.055	1.00 32.47	С
ATOM	1272	CG		A 172	34.168	13.298	11.539	1.00 36.36	С
ATOM	1273	CD		A 172	33.697	13.012	10.072	1.00 41.05	С
MOTA	1274	CE		A 172	34.338	11.721	9.543	1.00 44.14	С
ATOM	1275	NZ		A 172	34.321	11.571	8.024	1.00 49.11	N
ATOM	1276	N		A 173	33.099	16.900	14.316	1.00 31.59	N
ATOM	1277	CA		A 173	32.931	18.299	14.616	1.00 31.80	С
ATOM	1278	С		A 173	33.965	18.680	15.681	1.00 32.04	С
ATOM	1279	0	GLN	A 173	34.670	19.687	15.534	1.00 32.67	0
MOTA	1280	CB	GLN	A 173	31.522	18.581	15.117	. 1.00 31.45	С
ATOM	1281	CG	GLN	A 173	30.477	18.685	14.067	1.00 31.68	· c
MOTA	1282	CD		A 173	30.782	19.751	13.050	1.00 32.76	С
ATOM	1283			A 173	31.198		13.405	1.00 36.55	0
MOTA	1284	NE2	GLN	A 173	30.583		11.790	1.00 32.28	N
ATOM	1285			A 174	34.044		16.735	1.00 31.40	N
MOTA	1286			A 174	34.999		17.811	1.00 31.28	С
MOTA	1287	С	GLN	A 174	36.437	18.098	17.244	1.00 30.94	С
ATOM	1288		GLN	A 174	37.253		17.602		0
MOTA	1289	CB	GLN	A 174	34.808	16.971	18.861		С
MOTA	1290	CG	GLN	A 174	35.859	16.917	19.935	1.00 31.64	С
ATOM	1291	CD		A 174	35.704	15.717	20.836	1.00 31.52	С
ATOM	1292	OE1	LGLN	A 174	35.313	14.661			0
ATOM	1293		GLN	A 174	36.007				N
MOTA	1294	N	GLY	A 175	36.732				N
MOTA	1295			A 175	38.048				С
ATOM	1296			A 175	38.288				С
ATOM	1297			A 175	39.339				0
MOTA	1298			A 176	37.317				N
ATOM	1299			A 176	37.524				С
ATOM	1300	C		A 176	37.758		13.749	1.00 32.90	С
ATOM	1301	. 0		A 176	38.563		13.291	1.00 32.85	0

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1312	CG				34.716	22.947	15.353				2
1313	CD	ARG	A	177	34.728	23.721	14.062	1.00	37.56	(C
1314	NE	ARG	Α	177	33.704	23.135	13.222	1.00	42.96		N
1315	CZ	ARG	A	177	33.803	22.893	11.928				C
1316					34.897	23.218	11.247				N .
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1328							19.721				С
1329	CD2				34.054	22.115	19.769				С
1330	NE1				34.870	24.102	19.104	1.00	30.05		N
1331	CE2	TRP	Α	179	33.728	23.338	19.130	1.00	30.70		С
					33.067	21.145	19.902				С
					32.470	23.602	18.626				С
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1344	СВ					15.962	26.773				С
1345	CG	GLN	Į P	181	36.780	16.496	28.155	1.00	37.52		С
1346	CD						29.282				С
1347							29.442			•	0
											N
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1360	ō										ō
1361	СВ										C
1362							29.795				0
	1313 1314 1315 1316 1317 1318 1319 1320 1321 1322 1323 1324 1325 1326 1337 1333 1333 1333 1333 1333 1333 133	1303 CG 1304 CD 1305 CE 1306 NZ 1307 N 1308 CA 1309 C 1310 CB 1311 CB 1312 CG 1313 NE 1314 NE 1315 CZ 1316 NH1 1317 NH2 1318 N 1319 CA 1320 C 1321 O 1322 N 1323 CA 1324 C 1325 O 1326 CB 1327 CG 1328 CD1 1329 CD2 1330 NE1 1331 CE2 1332 CZ 1334 CZ 1335 CH2 1336 N 1337 CA 1338 C 1339 C 1331 CE2 1336 N 1337 CA 1338 C 1339 C 1340 N 1341 CA 1342 C 1343 C 1344 CB 1345 CG 1347 OE1 1347 OE1 1348 NE 1349 N 1350 CA 1351 C 1352 CD 1353 CB 1354 CG 1355 CD 1355 CD 1356 CD 1357 N 1358 CA 1359 C 1356 CD 1357 N 1358 CA 1359 C 1357 N 1358 CA 1359 C 1350 CB	1303 CG LYS 1304 CD LYS 1305 CE LYS 1306 NZ LYS 1307 N ARG 1308 CA ARG 1309 C ARG 1310 O ARG 1311 CB ARG 1312 CG ARG 1313 CD ARG 1314 NE ARG 1315 CZ ARG 1316 NH1 ARG 1317 NH2 ARG 1318 N GLY 1319 CA GLY 1320 C GLY 1321 O GLY 1321 O GLY 1322 N TRP 1323 CA TRP 1324 C TRP 1325 O TRP 1326 CB TRP 1327 CG TRP 1328 CD1 TRP 1329 CD2 TRP 1320 C GLY 1321 CE2 TRP 1322 CE3 TRP 1332 CE3 TRP 1333 CZ2 TRP 1334 CZ3 TRP 1335 CH2 TRP 1336 N GLY 1337 CA GLY 1338 C GLY 1338 C GLY 1339 O GLY 1336 N GLY 1337 CA GLY 1337 CA GLY 1338 C GLY 1339 C GLY 1334 CZ3 TRP 1335 CH2 TRP 1336 N GLY 1337 CA GLY 1337 CA GLY 1338 C GLY 1339 C GLY 1339 C GLY 1340 N GLN 1341 CA GLN 1342 C GLN 1344 CB GLN 1345 CG GLN 1347 OE1 GLN 1348 NE2 GLN 1349 N LEU 1350 CA LEU 1351 C LEU 1353 CB LEU 1353 CB LEU 1354 CG LEU 1355 CD1 LEU 1355 CD1 LEU 1356 CD2 LEU 1357 N THI 1358 CA THI 1358 CA THI 1358 CA THI 1359 C THI 1358 CA THI 1359 C THI 1358 CA THI 1359 C THI 1358 CA THI 1359 C THI 1358 CA THI 1359 C THI 1358 CA THI 1359 C THI 1358 CA THI 1359 C THI 1359 C THI 1350 C THI 1351 C LEU 1357 N THI 1358 CA THI 1358 CA THI 1359 C THI 1359 C THI 1350 C THI 1351 C LEU 1357 N THI 1358 CA THI 1359 C THI 1350 C THI 1351 C LEU 1357 N THI 1358 CA THI 1359 C THI 1359 C THI 1350 C THI 1351 C LEU 1357 N THI 1358 CA THI 1359 C THI 1350 C THI 1351 C LEU 1357 N THI 1358 CA THI 1359 C THI 1350 C THI 1351 C LEU 1357 N THI 1358 CA THI 1359 C THI 1359 C THI 1350 C THI 1350 C THI 1351 C LEU 1351 C LEU 1355 CD1 LEU 1357 N THI 1358 CA THI 1359 C THI 1350 C THI 1350 C THI 1351 C LEU 1351 C LEU 1355 CD1 LEU 1356 CD2 LEU 1357 N THI 1358 CA THI 1359 C THI 1350 C THI 1350 C THI 1351 C LEU 1351 C THI 1351	1303	1303 CG LYS A 176 1304 CD LYS A 176 1305 CE LYS A 176 1306 NZ LYS A 177 1307 N ARG A 177 1308 CA ARG A 177 1310 O ARG A 177 1311 CB ARG A 177 1312 CG ARG A 177 1313 CD ARG A 177 1314 NE ARG A 177 1315 CZ ARG A 177 1316 NH1 ARG A 177 1317 NH2 ARG A 177 1318 N GLY A 178 1320 C GLY A 178 1320 C GLY A 178 1321 O GLY A 178 1322 N TRP A 179 1323 CA TRP A 179 1324 C TRP A 179 1325 O TRP A 179 1326 CB TRP A 179 1327 CG TRP A 179 1328 CD1 TRP A 179 1329 CD2 TRP A 179 1329 CD2 TRP A 179 1330 NE1 TRP A 179 1330 NE1 TRP A 179 1331 CE2 TRP A 179 1332 CE3 TRP A 179 1333 CZ2 TRP A 179 1334 CZ3 TRP A 179 1335 CH2 TRP A 179 1336 N GLY A 180 1337 CA GLY A 180 1337 CA GLY A 180 1338 C GLY A 180 1339 O GLY A 180 1339 C GLY A 180 1331 CA GLY A 180 1334 CA GLY A 180 1335 CA GLY A 180 1336 C GLY A 180 1337 CA GLY A 180 1334 CA GLY A 180 1335 CA GLY A 180 1336 C GLY A 180 1337 CA GLY A 180 1337 CA GLY A 180 1338 C GLY A 180 1339 C GLY A 180 1341 CA GLN A 181 1342 C GLN A 181 1344 CB GLN A 181 1345 CG GLN A 181 1346 CD GLN A 181 1347 OE1 GLN A 181 1348 NE2 GLN A 181 1349 N LEU A 182 1350 CA LEU A 182 1351 C LEU A 182 1355 CD1 LEU A 182 1355 CD1 LEU A 182 1357 N THR A 183 1358 CA THR A 183 1359 C THR A 183 1359 C THR A 183	1303 CG LYS A 176 1304 CD LYS A 176 1305 CE LYS A 176 1306 NZ LYS A 176 1307 N ARG A 177 1308 CA ARG A 177 1309 C ARG A 177 1310 O ARG A 177 1311 CB ARG A 177 1312 CG ARG A 177 1313 CD ARG A 177 1315 CZ ARG A 177 1315 CZ ARG A 177 1316 NH1 ARG A 177 1317 NH2 ARG A 177 1317 NH2 ARG A 177 1318 N GLY A 178 1319 CA GLY A 178 1320 C GLY A 178 1321 O GLY A 178 1321 O GLY A 178 1322 N TRP A 179 1323 CA TRP A 179 1325 O TRP A 179 1326 CB TRP A 179 1327 CG TRP A 179 1328 CD1 TRP A 179 1329 CD2 TRP A 179 1320 CC TRP A 179 1321 CE3 TRP A 179 1322 CE3 TRP A 179 1323 CA TRP A 179 1324 CC3 TRP A 179 1325 CC3 TRP A 179 1326 CB TRP A 179 1327 CG TRP A 179 1328 CD1 TRP A 179 1329 CD2 TRP A 179 1330 NE1 TRP A 179 1331 CE2 TRP A 179 1331 CE2 TRP A 179 1332 CA TRP A 179 1333 CZ2 TRP A 179 1334 CZ3 TRP A 179 1335 CH2 TRP A 179 1336 N GLY A 180 1337 CA GLY A 180 1339 O GLY A 180 1339 O GLY A 180 1331 CA GLY A 180 1334 CZ3 TRP A 179 1335 CH2 TRP A 179 1336 N GLY A 180 1337 CA GLY A 180 1337 CA GLY A 180 1339 O GLY A 180 1340 N GLN A 181 1344 CB GLN A 181 1344 CB GLN A 181 1344 CB GLN A 181 1345 CG GLN A 181 1346 CD GLN A 181 1347 OE1 GLN A 181 1348 NE2 GLN A 181 1349 N LEU A 182 1350 CB LEU A 182 1351 CB LEU A 182 1353 CB LEU A 182 1353 CB LEU A 182 1355 CD1 LEU A 182 1356 CD2 LEU A 182 1357 N THR A 183 1358 CA THR A 183 1359 C THR A 183 1359 C THR A 183 1359 C THR A 183 1350 O THR A 183 1350 CD THR A 183 1350 C THR A 183 1350 C THR	1303 CG LYS A 176 1304 CD LYS A 176 1305 CE LYS A 176 1306 NZ LYS A 176 1307 N ARG A 177 1308 CA ARG A 177 1309 C ARG A 177 1310 O ARG A 177 1311 CB ARG A 177 1311 CB ARG A 177 1312 CG ARG A 177 1313 CD ARG A 177 1313 CD ARG A 177 1314 NE ARG A 177 1315 CZ ARG A 177 1316 NH1 ARG A 177 1317 1316 CA ARG A 177 1317 1318 CD ARG A 177 1318 NE ARG A 177 1319 CZ ARG A 177 1319 CZ ARG A 177 1311 CB ARG A 177 1311 CB ARG A 177 1312 CB ARG A 177 1313 CD ARG A 177 1313 CD ARG A 177 1314 NE ARG A 177 1315 CZ ARG A 177 1316 NH1 ARG A 177 1317 1316 NH1 ARG A 177 1317 1318 N GLY A 178 1319 CA GLY A 178 1320 C GLY A 178 1321 O GLY A 178 1322 C TRP A 179 1323 CA TRP A 179 1324 C TRP A 179 1325 C TRP A 179 1326 CB TRP A 179 1327 CG TRP A 179 1328 CD1 TRP A 179 1329 CD2 TRP A 179 1329 CD2 TRP A 179 1330 NE1 TRP A 179 1331 CE2 TRP A 179 1331 CE2 TRP A 179 1332 CA TRP A 179 1333 CE2 TRP A 179 1334 CZ2 TRP A 179 1335 CH2 TRP A 179 1336 CB LY A 180 1337 CA GLY A 180 1339 C GLY A 180 1331 CE3 TRP A 179 1336 CB CB TRP A 179 1337 CA GLY A 180 1338 C GLY A 180 1339 C GLY A 180 1331 CE3 TRP A 179 134.60 1344 CB GLN A 181 1344 CB GLN A 181 1344 CB GLN A 181 1345 CG GLN A 181 1347 CG GLN A 181 1348 NE CG GLN A 181 1349 N LEU A 182 1355 CD LEU A 182 1355 CD LEU A 182 1355 CD LEU A 182 1355 CD LEU A 182 1355 CD LEU A 182 1357 N THR A 183 1358 CA THR A 183 1359 C THR A 183 1350 C THR A 183 1355 CD THR A 183 1355 CD THR A 183 1356 CD THR A 183 1357 CR THR A 183 1358 CA THR A 183 1359 C THR A 183 1350 CA THR A 183 1350 CA THR A 183 1351 CB LEU A 182 1355 CD1 LEU A 182 1357 N THR A 183 1358 CA THR A 183 1359 C THR A 183 1360 O TH	1303 CG	1303 CG	1303 CG LYS A 176 1304 CD LYS A 176 1306 NZ LYS A 176 1307 N ARG A 177 1308 CA ARG A 177 1309 C ARG A 177 1309 C ARG A 177 1309 C ARG A 177 1309 C ARG A 177 1309 C ARG A 177 1301 CB ARG A 177 1301 CB ARG A 177 1301 CB ARG A 177 1302 CG ARG A 177 1303 CD ARG A 177 1303 CD ARG A 177 1303 CD ARG A 177 1303 CD ARG A 177 1304 CD ARG A 177 1305 CE ARG A 177 1305 CE ARG A 177 1306 CA ARG A 177 1307 N ARG A 177 1308 CA ARG A 177 1309 C ARG A 177 1309 C ARG A 177 1309 C ARG A 177 1309 C ARG A 177 1301 CB ARG A 177 1301 CB ARG A 177 1301 CB ARG A 177 1301 CD ARG A 177 1301 CD ARG A 177 1301 CD ARG A 177 1301 CD ARG A 177 1301 CD ARG A 177 1301 CD ARG A 177 1301 CD ARG A 177 1301 CD ARG A 177 1301 CD ARG A 177 1301 CD ARG A 177 1301 CD ARG A 177 1301 CD ARG A 177 1301 CD ARG A 177 1302 CD ARG A 177 1303 CD ARG A 177 1304 NC ARG A 177 1305 CD ARG A 177 1306 NC LYS A 178 1307 NH2 ARG A 177 1308 N GLY A 178 1309 C GLY A 178 1300 C GLY A 178 1300 C GLY A 178 1301 CD ARG A 179 1302 C GLY A 178 1302 C GLY A 178 1303 CD TRP A 179 1303 CD TRP A 179 1304 CD TRP A 179 1305 CD TRP A 179 1306 CD TRP A 179 1307 NH2 ARG A 179 1307 NH2 ARG A 179 1308 CD ARG A 177 1309 CD TRP A 179 1309 CD	1303 CG LYS A 176 34.982 19.185 10.168 1.00 39.44 1305 CE LYS A 176 34.982 19.185 10.168 1.00 39.44 C 1306 NZ LYS A 176 34.085 18.032 9.961 1.00 40.94 C 1307 N ARG A 177 37.074 21.398 1.00 45.01 N. 1308 CA ARG A 177 37.074 21.398 1.00 32.98 N 1309 CA ARG A 177 38.313 22.713 16.678 1.00 33.16 C 1310 O ARG A 177 38.453 23.717 17.370 1.00 33.61 C 1311 CB ARG A 177 38.453 23.717 17.370 1.00 33.01 C 1312 CG ARG A 177 38.453 22.713 16.678 1.00 33.16 C 1313 CD ARG A 177 38.453 22.947 15.553 1.00 35.87 1313 CD ARG A 177 34.728 23.721 14.062 1.00 37.56 1314 NE ARG A 177 33.032 22.993 11.928 1.00 45.93 1315 CZ ARG A 177 33.803 22.893 11.928 1.00 45.93 1315 CZ ARG A 177 32.770 22.349 11.304 1.00 47.47 1318 N GLY A 178 40.068 21.629 17.907 1.00 31.78 1320 C GLY A 178 40.068 21.629 17.907 1.00 31.78 1321 O GLY A 178 40.068 21.629 17.907 1.00 31.78 1322 N TRP A 179 38.223 21.380 19.468 1.00 30.56 1323 C ARP A 179 38.223 21.380 19.468 1.00 30.56 1324 C TRP A 179 38.282 20.385 21.789 1.00 30.44 1325 C GRP A 179 39.098 19.464 21.416 1.00 29.50 1326 C B TRP A 179 36.200 21.115 20.806 1.00 30.54 1327 C G TRP A 179 36.200 21.115 20.806 1.00 30.54 1328 C C TRP A 179 36.200 21.115 20.806 1.00 30.54 1329 C TRP A 179 36.200 21.115 20.806 1.00 30.54 1329 C TRP A 179 36.200 21.115 20.806 1.00 30.54 1329 C TRP A 179 36.200 21.115 20.806 1.00 30.36 1321 O G TRP A 179 36.200 21.115 20.806 1.00 30.54 1322 C TRP A 179 36.200 21.115 20.806 1.00 30.54 1324 C TRP A 179 36.200 21.115 20.806 1.00 30.55 1325 C G TRP A 179 36.200 21.115 20.806 1.00 30.59 1326 C G TRP A 179 36.200 21.115 20.806 1.00 30.59 1327 C G TRP A 179 36.200 21.115 20.806 1.00 30.59 1328 C C TRP A 179 36.200 21.115 20.806 1.00 30.55 1329 C C TRP A 179 36.200 21.115 20.806 1.00 30.50 1329 C C TRP A 179 36.200 21.115 20.806 1.00 30.50 1320 C TRP A 180 36.607 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

ATOM	1363		THR P				33.764	19.178	29.846	1.00			C
MOTA	1364	N	SER P				30.005	16.673	29.355		28.14		N
MOTA	1365	.CA	SER F				28.734	16.144	29.805		28.16		C
MOTA	1366	С	SER A				27.602	16.374	28.878		28.07		C
ATOM	1367	0	SER A				27.703	17.120	27.931		29.72		0
MOTA	1368	CB	SER A				28.357	16.750	31.149		27.81		C 0
MOTA	1369	OG	SER A				28.166	18.132	31.017		30.35 27.93		И
ATOM	1370	N	ASN A				26.505 25.288	15.721 15.850	29.176 28.434		28.66		C
ATOM	1371 1372	CA.	ASN A				24.235	16.086	29.476		28.67		C
ATOM ATOM	1373	С 0	ASN A				23.974	15.226	30.291		27.67		Õ
ATOM	1374	CB	ASN A				24.927	14.543	27.683		28.53		c
ATOM	1375	CG	ASN A				25.914	14.191	26.589		29.19		c
ATOM	1376		ASN A				26.684	13.278	26.766		30.93	•	Ō
ATOM	1377		ASN A				25.891	14.910	25.451		29.67		N
ATOM	1378	N	LEU				23.583	17.221	29.415		29.39		N
ATOM	1379	CA	LEU .				22.557	17.526	30.388		30.47		С
MOTA	1380	C	LEU .				21.179	17.177	29.835		30.85		С
ATOM	1381	O	LEU			-	20.796	17.566	28.714	1.00	30.64		0
ATOM	1382	СВ	LEU				22.617	18.998	30.730	1.00	30.48	•	С
MOTA	1383	CG	LEÙ .	A :	186		21.779	19.484	31.917	1.00	32.51		С
MOTA	1384	CD1	LEU	A	186		22.330	18.952	33.238	1.00	31.55		С
MOTA	1385	CD2	LEU	Α	186		21.678	21.072	31.954	1.00	29.96		С
ATOM	1386	N	LEU				20.409	16.439	30.613		31.21		N
MOTA	1387	CA	LEU	A	187		19.042	16.155	30.188		30.60		С
ATOM	1388	С	LEU	Α	187		18.162	17.256	30.787		30.79		С
MOTA	1389	0	LEU				18.257	17.557	31.991		29.69		0
MOTA	1390	CB	LEU				18.626	14.781	30.644		30.50		C
MOTA	1391	CG	LEU				17.130	14.465	30.590		32.29		С
MOŢA	1392		LEU				16.592	14.409	29.164		33.95		C
MOTA	1393	CD2					16.864	13.137	31.270		32.62		C
MOTA	1394	N	LEU				17.390	17.933	29.939		30.75		N
ATOM	1395	CA	LEU				16.513	18.973	30.426		31.42		C
ATOM	1396	С	LEU				15.053	18.646	30.107		32.02		C
ATOM	1397	0	LEU				14.676	18.481	28.941		31.44	•	O C
ATOM	1398	CB	LEU				16.856	20.323	29.821		31.69		c
MOTA	1399	CG	LEU				18.253	20.823	30.131 28.904		32.24 32.79		C
MOTA	1400	CD1					19.094	22.200	30.658		32.79		C
ATOM ATOM	1401 1402	CD2	LEU				18.121 14.228	18.568	31.146		32.26		N
MOTA	1402	CA	ILE				12.816	18.305	30.944		32.23		C
MOTA	1403	C			189		12.067	19.386			32.02		C
ATOM	1405	Ö			189		12.194	19.520			31.42		ō
ATOM	1406	CB			189		12.427	16.966			32.05		Ċ
ATOM	1407		LILE				13.256	15.894			33.02		C
ATOM	1408		2 ILE				10.957	16.764			32.90		С
ATOM	1409		LILE				13.006	14.466			34.20		С
ATOM	1410				190		11.279	20.145			31.94		N
ATOM	1411				190		10.623	21.334			31.49		С
ATOM	1412				190		9.147	21.362			31.41		С
ATOM	1413				190		8.671	20.649			30.40		0
ATOM	1414				191		8.433			1.00	0 31.55		N
ATOM	1415				191		7.027	22.378		1.0	0 32.41		C
ATOM	1416				191		6.863			1.0	0 32.03		С
MOTA	1417				191		7.722			1.0	0 32.29		0
MOTA	1418				191		6.313	22.672	33.008		0 33.21		С
MOTA	1419	CG	MET	Α	191		6.294				0 35.09		С
MOTA	1420		MET	Α	191		5.828				0 39.51		S
MOTA	1421				191		4.213				0 39.52		С
MOTA	1422				192		5.755				0 31.96		N
MOTA	1423	CA	GLU	J A	192		5.459	24.588	29.081	1.0	0 32.31	•	С

ATOM	1424	С	GLU	A	192	5.511	25.919	29.776	1.00 31.73	С
ATOM	1425	0	GLU			5.096	26.041	30.913	1.00 31.73	Ö
MOTA	1426	CB	GLU			4.087	24.375	28.508	1.00 33.09	č
ATOM	1427	CG	GLU			2.995	24.434	29.552	1.00 34.74	Č
ATOM	1428	CD	GLU			1.679	23.940	29.019	1.00 36.73	č
ATOM	1429	OE1				1.630	23.515	27.832	1.00 37.30	. 0
MOTA	1430		GLU			0.698	24.001	29.791	1.00 38.64	Ö
MOTA	1431	N	GLY			6.049	26.926	29.103	1.00 30.04	. И
MOTA	1432	CA	GLY			6.201	28.242	29.714	1.00 30.87	C
MOTA	1433	С	GLY			7.480	28.432	30.521	1.00 30.28	Č
MOTA	1434	0	GLY			7.777	29.534	30.901	1.00 30.29	Ö
ATOM	1435	N	ASN			8.223	27.375	30.825	1.00 29.85	N
ATOM	1436	CA	ASN			9.460	27.536	31.604	1.00 29.38	C
MOTA	1437	С	ASN			10.473	28.371	30.840	1.00 28.61	c
MOTA	1438	0	ASN			10.606	28.216	29.615	1.00 28.58	Ö
ATOM	1439	СВ	ASN			10.136	26.186	31.866	1.00 29.15	Č
ATOM	1440	CG	ASN			9.565	25.445	33.049	1.00 29.50	C
ATOM	1441	OD1	ASN			8.632	25.896	33.714	1.00 32.61	Ö
MOTA	1442		ASN			10.146	24.305	33.334	1.00 28.53	Ŋ
ATOM	1443	N	VAL			11.221	29.194	31.561	1.00 27.70	N
ATOM	1444	CA	VAL			12.272	29.998	30.962	1.00 27.80	C
MOTA	1445	С	VAL			13.586	29.858	31.701	1.00 27.07	Č
MOTA	1446	0	VAL			13.636	29.898	32.939	1.00 27.43	Ō
MOTA	1447	CB	VAL	Α	195	11.904	31.520	31.018	1.00 28.18	C
MOTA	1448	CG1				13.056	32.371	30.560	1.00 26.78	C
MOTA	1449	CG2	VAL	A	195	10.662	31.789	30.187	1.00 29.06	Ċ
ATOM	1450	N	THR	Α	196	14.659	29.712	30.953	1.00 26.48	Ŋ
ATOM	1451	CA	THR	Α	196	15.994	29.811	31.530	1.00 26.08	C
ATOM	1452	С	THR	Α	196	16.462	31.184	31.084	1.00 27.03	C
MOTA	1453	0	THR	A	196	16.614	31.425	29.876	1.00 26.51	Ō
MOTA	1454	CB	THR	Α	196	16.915	28.811	30.934	1.00 25.96	
MOTA	1455	OG1	THR	Α	196	16.525	27.478	31.309	1.00 26.20	
MOTA	1456	CG2	THR	Α	196	18.340	29.012	31.457	1.00 23.99	
MOTA	1457	N	PRO	Α	197	16.647	32.090	32.036	1.00 27.21	N
ATOM	1458	CA	PRO	Α	197	17.053	33.451	31.725	1.00 27.46	
MOTA	1459	C			197	18.432	33.512	31.113	1.00 27.48	
MOTA	1460	0			197	19.248	32.588	31.293	1.00 27.52	
MOTA	1461	CB	PRO	A	197	17.007	34.166	33.075	1.00 27.56	
MOTA	1462	CG	PRO	Α	197	16.226	33.344 ·	33.924	1.00 28.15	С
MOTA	1463	CD	PRO	A	197	16.384	31.914	33.470	1.00 27.92	С
MOTA	1464	N	ALA	Α	198	18.668	34.616	30.413	1.00 26.77	N
MOTA	1465	CA			198	19.877	34.830	29.647	1.00 26.92	С
ATOM	1466	С			198	21.172	34.681	30.438	1.00 27.14	
MOTA	1467	0			198	21.354	35.278	31.520	1.00 25.53	
ATOM	1468	CB			198	19.828	36.235	29.021	1.00 27.07	C
MOTA	1469	N			199	22.091	33.929	29.839	1.00 27.28	
MOTA	1470	CA			199	23.399	33.673	30.424	1.00 27.81	
ATOM	1471	C			199	24.319	33.208	29.333	1.00 28.09	
ATOM	1472	0			199	23.857	32.933	28.197	1.00 28.34	
MOTA	1473	CB			199	23.323	32.549	31.461	1.00 27.10	
ATOM	1474	CG			199	22.963	31.221	30.864	1.00 29.70	
MOTA	1475		HIS			21.668	30.891	30.525	1.00 30.01	
ATOM	1476		HIS			23.728	30.180	30.463	1.00 29.60	
MOTA	1477		HIS			21.647	29.684	29.993	1.00 29.66	
ATOM	1478		HIS			22.881	29.236	29.926	1.00 30.43	
ATOM	1479	N			200	25.612	33.104	29.671	1.00 28.30	
ATOM	1480	CA			200	26.607	32.518	28.769	1.00 28.15	
ATOM	1481	C			200	27.298	31.351	29.482	1.00 27.91	
ATOM	1482	0			200	27.335	31.333	30.690	1.00 27.87	
ATOM	1483	CB			200	27.585	33.534	28.217	1.00 28.02	
ATOM	1484	CG	TIR	A	200	28.540	34.142	29.226	1.00 29.58	С

ATOM	1485	CD1	TYR	A	200	29.784	33.571	29.462	1.00 28.14	С
MOTA	1486	CD2	mvn	7	200 .					
		_	TYR			28.231	35.342	29.871	1.00 29.32	С
MOTA	1487	CE1	TYR	Α	200	30.660	34.128	30.367	1.00 30.20	С
ATOM	1488									
			TYR			29.107	35.919	30.777	1.00 29.61	С
ATOM	1489	CZ	TYR	Α	200	30.319	35.315	31.031	1.00 29.78	С
ATOM	1490	ОН	TYR							
		On				31.180	35.864	31.940	1.00 24.43	0
MOTA	1491	N	ASP	Α	201	27.797	30.363	28.727	1.00 27.73	N
ATOM	1492	CA								
			ASP			28.461	29.180	29.302	1.00 27.65	С
ATOM	1493	С	ASP	Α	201	29.873	29.220	28.799	1.00 27.87	С
MOTA	1494	0	ASP							
		U				30.080	29.765	27.768	1.00 27.68	0
MOTA	1495	CB	ASP	Α	201	27.775	27.884	28.855	1.00 26.32	С
ATOM	1496	CG								
			ASP			26.356	27.768	29.363	1.00 25.12	С
ATOM	1497	OD1	ASP	Α	201	26.156	27.722	30.605	1.00 23.49	0
ATOM	1498									
			ASP			25.360	27.687	28.589	1.00 27.18	0
ATOM	1499	N	GLU	Α	202	30.843	28.682	29.520	1.00 29.28	N
MOTA	1500	CA								
			GLU			32.228	28.672	29.013	1.00 31.18	С
ATOM	1501	С	GLU	Α	202	32.571	27.435	28.190	1.00 31.54	С
ATOM	1502	0	GLU							
						33.734	27.060	28.139	1.00 33.48	. 0
MOTA	1503	CB	GLU	A	202	33.250	28.741	30.155	1.00 30.78	C
ATOM	1504	CG	GLU	Δ	202 .	33.122	29.981	31.003	1.00 33.61	C
ATOM	1505	CD	GLU			34.194	30.081	32.062	1.00 35.96	. C
MOTA	1506	OE1	GLU	Α	202	34.036	29.531	33.166	1.00 41.25	·o
ATOM	1507	OE2								
		OEZ	GLU			35.199	30.718	31.788	1.00 39.13	0
MOTA	1508	N	GLN	A	203	31.582	26.747	27.641	1.00 31.19	N
MOTA	1509	CA	GLN			31.844				
							25.589	26.833	1.00 30.78	C
MOTA	1510	С	GLN	Α	203	31.078	25.743	25.556	1.00 29.96	С
MOTA	1511	0	GLN	Δ	203	30.213	26.581	25.462	1.00 30.22	
										0
ATOM	1512	CB	GLN			31.427	24.315	27.546	1.00 31.32	С
ATOM	1513	CG	GLN	Α	203	32.364	23.971	28.725	1.00 34.97	. С
MOTA	1514	CD	GLN							9
						32.204	22.548	29.288	1.00 35.23	С
MOTA	1515	OE1	GLN	Α	203	32.161	21.559	28.551	1.00 36.82	0
MOŤA	1516	NE2	GLN	Δ	203	32.160	22.456	30.600	1.00 35.56	
										N
MOTA	1517	N	GLN	Α	204	31.461	24.961	24.555	1.00 29.46	N
ATOM	1518	CA	GLN	Α	204	30.791	24.911	23.292	1.00 28.65	С
ATOM	1519	С								C
					204	29.641	23.941	23.494	1.00 28.27	С
MOTA	1520	0	GLN	Α	204	29.797	22.941	24.194	1.00 27.65	. 0
ATOM	1521	CB			204					
						31.717	24.381	22.214	1.00 29.02	С
ATOM	1522	CG	GLN	Α	204	33.006	25.154	22.028	1.00 28.50	C
ATOM	1523	CD	GT.N	Δ	204	32.818	26.366			Š
								21.150	1.00 27.16	С
MOTA	1524	OFT	GLN			31.690	26.742	20.846	1.00 22.90	0
MOTA	1525	NE2	GLN	Α	204	33.921	26.952	20.714	1.00 23.20	N
ATOM	1526	N			205					
		-				28.497	24.219	22.864	1.00 27.36	N
MOTA	1527	CA	ASN	Α	205	27.302	23.424	23.058	1.00 27.13	С
MOTA	1528	С	N C N	7\	205	26.552	23.052	21.777		
									1.00 27.39	С
ATOM	1529	0	ASN	A.	205	26.151	23.930	20.999	1.00 27.36	0
MOTA	1530	CB	ASN	Δ	205 ·	26.378	24.229	23.967		
									1.00 26.95	С
MOTA	1531	CG			205	25.083	23.525	24.327	1.00 27.30	С
MOTA	1532	OD1	ASN	Α	205 ·	24.726	22.453	23.818	1.00 27.11	0
MOTA	1533									
			ASN			24.319	24.190	25.171	1.00 24.64	N
MOTA	1534	N	PHE	Α	206	26.383	21.749	21.542	1.00 26.46	N
ATOM	1535	CA			206	25.417	21.334			
								20.554	1.00 25.88	С
MOTA	1536	С			206	24.181	20.946	21.373	1.00 25.65	С
MOTA	ັ1537	0	PHE	Α	206	24.230	19.988	22.178	1.00 25.16	0
ATOM	1538									
		CB			206	25.909	20.170	19.717	1.00 26.28	С
MOTA	1539	CG	PHE	Α	206	26.837	20.566	18.636	1.00 24.81	· c
ATOM	1540		PHE			26.416				
							21.374	17.633	1.00 26.27	С
MOTA	1541		PHE			28.122	20.098	18.616	1.00 25.53	C
MOTA	1542	CE1	PHE	Α	206	27.248	21.736	16.634	1.00 27.05	C
ATOM	1543		PHE							
						28.991	20.469	17.617	1.00 26.80	С
MOTA	1544	CZ	PHE	Α	206	28.549	21.274	16.619	1.00 28.34	С
ATOM	1545	N	PHF	А	207	23.084	21.648	21.086		
					_ 0,	23.004	21.040	51.000	1.00 25.08	N

							•			•	•
ATOM	1546	CA	PHE A 2	207	21.809	21.625	21.827	1.00 25.52			С
ATOM	1547	С	PHE A 2		20.775	20.885	21.011	1.00 25.55			С
MOTA	1548	0	PHE A 2	207	20.261	21.410	20.058	1.00 25.61			0
MOTA	1549	CB	PHE A 2	207		23.107	22.074	1.00 25.37			C
ATOM	1550	CG	PHE A 2	207		23.346	22.872	1.00 23.70			C
MOTA	1551		PHE A			23.547	22.234	1.00 24.08			С
ATOM	1552		PHE A		20.199		24.220	1.00 25.24			C
MOTA	1553		PHE A		17.800		22.927	1.00 24.50			C
MOTA	1554		PHE A		19.035		24.959	1.00 26.04			C
MOTA	1555	CZ	PHE A		17.836		24.298	1.00 26.68			C
MOTA	1556	N	ALA A		20.490		21.422	1.00 26.60			N
MOTA	1557	CA	ALA A		19.667		20.689	1.00 26.45		•	C
MOTA	1558	С	ALA A		18.231		21.210	1.00 27.10			0
MOTA	1559	0	ALA A		17.966	17.987	22.273	1.00 26.47			C
MOTA	1560	CB	ALA A		20.303	17.363 19.121	20.766 20.419	1.00 25.67 1.00 27.02			1/2
ATOM	1561	N	GLN A		17.306	19.125	20.419	1.00 27.02			Ċ
ATOM	1562	CA	GLN A		15.918 15.276	17.781		1.00 27.55			Ċ
ATOM	1563 1564	Ċ	GLN A GLN A		15.489	17.190	19.427	1.00 26.51			Ċ
ATOM	1565	о Св	GLN A		15.195	20.301	20.179	1.00 27.15			Č
MOTA MOTA	1566	CG	GLN A		13.806	20.508	20.662	1.00 27.77			Č
ATOM	1567	CD	GLN A		13.740	20.959	22.126	1.00 29.40			(
MOTA	1568		GLN A		14.773	21.166		1.00 27.27			(
ATOM	1569		GLN A		12.517	21.118		1.00 27.15			ì
MOTA	1570	N	ILE A.		14.461			1.00 28.32			1
ATOM	1571	CA			13.897	15.998		1.00 29.37			(
MOTA	1572	C	ILE A		12.403	15.966	21.435	1.00 30.37			(
MOTA	1573	0	ILE A		11.849	15.275	20.619	1.00 31.58			(
ATOM	1574	СВ	ILE A	210	14.413	15.204		1.00 29.80			(
MOTA	1575	CG:	L ILE A	210	15.830	14.734		1.00 30.27			(
MOTA	1576		2 ILE A		13.525	14.005		1.00 30.25			'
MOTA	1577	CD:	I ILE A		16.624			1.00 32.28			
MOTA	1578	N	LYS A		11.757	16.664		1.00 31.18			
MOTA	1579				10.300	16.723		1.00 31.16			
MOTA	1580		LYS A		9.887	18.137					
MOTA	1581		LYS A		10.495	18.800					
MOTA	1582				9.767	15.891					
MOTA	1583				8.240						
MOTA	1584				7.787						
ATOM	1585				6.497	14.755					
ATOM			LYS A GLY A		8.844	18.592))		
MOTA MOTA	1587 1588				8.337						
MOTA	1589		GLY A		9.209						
ATOM	1590		GLY A		10.167						
MOTA	1591		TYR A		8.857						
ATOM	1592				9.507						
MOTA	. 1593		TYR A		10.046						
MOTA	1594				9.411						
ATOM	1595				8.502						
ATOM	1596				8.103						
MOTA	159		O1 TYR A		7.089			1.00 38.3	7		
ATOM	1598		2 TYR A		8.758						
ATOM	159		El TYR A		6.765				7		
MOTA	160		E2 TYR A		8.443		2 16.792				
ATOM	160			A 213	7.460						
ATOM	160			A 213	7.232	20.603					
ATOM	160			A 214	11.260	24.78					
MOTA	160			A 214	11.886						
MOTA	160			A 214	12.305						
ATOM	160	6 0	LYS I	A 214	12.91	26.83	3 20.695	5 1.00 31.8	4		

ATOM	1607	CB :	LYS A 21	. 4	13.112	25.244	23.311	1.00 3	1.08		С
ATOM	1608		LYS A 21		12.806	24.432	24.557	1.00 3	30.96		С
ATOM	1609		LYS A 21		14.106	23.949	25.159	1.00 3	30.84		С
ATOM	1610		LYS A 21		13.982	23.555	26.584	1.00 2			С
ATOM	1611		LYS A 21		15.278	23.118	27.162	1.00 2			N
			ARG A 21		11.992	28.193	22.241	1.00 3			N
ATOM	1612					29.385		1.00 2			C
ATOM.	1613		ARG A 21		12.445		21.549				C
MOTA	1614		ARG A 21		13.764	29.790	22.154	1.00 2			
ATOM	1615		ARG A 21		13.850	29.982	23.349	1.00 2			0
MOTA	1616		ARG A 21		11.431	30.502	21.690	1.00			С
ATOM	1617	CG	ARG A 21	15	11.835	31.810	21.004	1.00 2			C
ATOM	1618	CD	ARG A 21	15	11.221	32.960	21.731	1.00	32.78		C
ATOM	1619	NE	ARG A 21	1.5 ·	11.211	34.189	20.975	1.00	33.81		N
ATOM	1620		ARG A 2		10.540	35.259	21.336	1.00	35.12		С
ATOM	1621		ARG A 2		9.828	35.262	22.441	1.00			N
ATOM	1622		ARG A 2		10.586	36.338	20.581	1.00			N
ATOM	1623	N	CYS A 2		14.791	29.909	21.327	1.00			N
ATOM	1624	CA	CYS A 2		16.129	30.237	21.797		29.64		c
					16.533	31.603	21.274		30.06		C;
ATOM	1625	C	CYS A 2				20.092		31.32	•	0
MOTA	1626	0	CYS A 2		16.516	31.807					-
MOTA	1627	CB	CYS A 2		17.113	29.183	21.275		29.78		C
MOTA	1628	SG	CYS A 2		16.658	27.438	21.641		30.35	-	S
MOTA	1629	N	ILE A 2		16.849	32.556	22.149		30.28		N
ATOM	1630	CA	ILE A 2	17	17.303	33.876	21.744		29.78		С
ATOM	1631	С	ILE A 2	17	18.758	34.017	22.203	1.00	29.42		C.
ATOM	1632	0	ILE A 2	17	19.050	33.852	23.385	1.00	28.77		0
ATOM	1633	CB	ILE A 2		16.427	34.969	22.391	1.00	30.51		С
MOTA	1634		ILE A 2		14.934	34.705	22.111	1.00	31.29		С
ATOM	1635		ILE A 2		16.785	36.313	21.843		30.11		С
ATOM	1636		ILE A 2		14.009	35.655	22.847		33.08		С
MOTA	1637	N	LEU A 2		19.647	34.326	21.257		28.60		N
	1638	CA	LEU A 2		21.059	34.392	21.501		28.59		C
MOTA							21.257		28.74		č
MOTA	1639	C	LEU A 2		21.606	35.781					0
MOTA	1640	0	LEU A 2		21.102	36.522	20.412		29.64		C
MOTA	1641	СВ	LEU A 2		21.788	33.422	20.574		28.52		
MOTA	1642	CG	LEU A 2		21.927	31.980	21.028		28.46		C
MOTA	1643		LEU A 2		20.569	31.318	21.233		28.95		С
MOTA	1644	CD2	LEU A 2		22.707	31.196			27.94		С
ATOM	1645	N	PHE A 2	219	22.659	36.145			28.61		
MOTA	1646	CA	PHE A 2	219	23.309	37.458	21.774		28.07		C
MOTA	1647	С	PHE A 2	219 .	24.811	37.221	21.710		28.25		C
MOTA	1648	0	PHE A 2	2.19	25.352	36.468	22.517	1.00	28.82		0
MOTA	1649		PHE A 2		22.987	38.415			26.73		C
ATOM	1650		PHE A 2		21.522	38.553			27.28		С
ATOM	1651		PHE A		20.874	37.658			25.73		С.
ATOM	1652		PHE A		20.782	39.598			28.57		С
MOTA	1653		L PHE A		19.536				26.59		C
					19.443				27.78		č
MOTA	1654		PHE A								č
ATOM	1655		PHE A		18.816				28.22		и∙
ATOM	1656		PRO A		25.501				28.30		
MOTA	1657				26.946				28.76		C
MOTA	1658		PRO A		27.688				29.07		C
MOTA	1659		PRO A		27.172				29.11		0
MOTA	1660	CB	PRO A	220	27.336				28.79		C
ATOM	1661	. CG	PRO A	220	26.016				29.65		С
MOTA	1662	CD	PRO A	220	24.987	38.794	19.790	1.00	28.85		С
MOTA	1663		PRO A		28.914				29.09		N
MOTA	1664				29.725				28.85		C
ATOM	1665		PRO A		29.979				28.60		С
ATOM	1666		PRO A		30.223				26.85		0
ATOM	1667				31.018				29.01		C
AIOM	1001		IIO A		52.520	0					-

ATOM	1668	CG	PRO	Α	221	30.665	36.286	22.114	1.00 3	0.46		С
MOTA	1669	CD	PRO	A	221	29.580		21.232	1.00 2			č
ATOM	1670	N .	ASP	Α	222	29.853		22.062	1.00 2			N
MOTA	1671	CA	ASP	Α	222	30.155		22.044	1.00 2			Ċ
MOTA	1672	С	ASP	Α	222	28.976		22.533	1.00 2			Č
MOTA	1673	0	ASP	Α	222	28.948		22.432	1.00 3		•	Ö
MOTA	1674	CB	ASP			30.631		20.693	1.00 2			c
MOTA	1675	CG.	ASP			29.541		19.655	1.00 3			Ċ
MOTA	1676	OD1	ASP			28.368		19.920		0.56		Ö
MOTA	1677		ASP			29.785		18.495		9.36		ŏ
ATOM '	1678	N	GLN			28.000		23.083		9.33		N
ATOM	1679	CA	GLN			26.902		23.676	1.00 2			C
MOTA	1680	С	GLN			27.012		25.194		8.97		C
MOTA	1681	0	GLN			26.065		25.919	1.00 2			Ö
MOTA	1682	СВ	GLN			25.575		23.110		0.22	•	C
ATOM	1683	CG	GLN			25.244		21.762	1.00 3			C
MOTA	. 1684	CD	GLN			23.866		21.241		37.71		C
MOTA	1685	OE1	GLN			22.899		22.005	1.00 4			Ö
ATOM	1686	NE2				23.760		19.943		8.91		N
MOTA	1687	N	PHE			28.181		25.672	1.00 2			N
MOTA	1€88	CA	PHE			28.452		27.115	1.00 2			C
ATOM	1689	С	PHE			27.932	•	27.771		9.27		C
ATOM	1690	0 :	PHE			27.248		28.786	1.00 2			0
ATOM	1691	CB	PHE			29.968		27.373	1.00 2			c
MOTA	1692	CG	PHE			30.338		28.810	1.00 2		•	C
ATOM	1693		PHE			30.526		29.619	1.00 2			C
MOTA	1694		PHE			30.560		29.365		25.77		C
ATOM	1695		PHE			30.878		30.930	1.00 2			C
ATOM	1696		PHE			30.928		30.675	1.00 2			C
MOTA	1697	CZ	PHE			31.056		31.467	1.00 2			c
ATOM	1698	N	GLU			28.253		27.177	1.00 3			N
ATOM	1699	CA	GLU			27.873		27.753	1.00 3			C
MOTA	1700	С			225	26.362		27.709	1.00 3			C
ATOM	1701	0			225	25.925		28.738	1.00 2			Ö
ATOM	1702	СВ	GLU			28.401		26.927	1.00 2			C
MOTA	1703	CG			225	29.894		27.083	1.00 3			C
MOTA	1704	CD			225	30.327			1.00 4			C
ATOM	1705		GLU			29.848		28.389	1.00 4			Ö
MOTA	1706		GLU			. 31.230		26.665	1.00 5			Ö
ATOM	1707	N			226	25.579		27.116	1.00 2			N
MOTA	1708	CA			226	24.132		27.155	1.00 2			C
MOTA	1709	С			226	23.429		28.056	1.00 2			Č
MOTA	1710	0			226	22.236		28.352	1.00 2			Ö
MOTA	1711	СВ			226	23.541		25.767	1.00 2			č
MOTA	1712	SG			226	24.193		24.441	1.00 2			s
MOTA	· 1713	N			227	24.133		28.483	1.00 2			N
MOTA	1714	CA			227	23.469		29.242	1.00 2			Ĉ
MOTA	1715	С			227	23.760		30.737	1.00 2			č
MOTA	1716	0			227			31.465	1.00 2			ō
MOTA	1717	CB			227	23.701		28.531	1.00 2			Č
MOTA	1718	CG			227	22.853		27.246	1.00 3			Ċ
MOTA	1719	CD1	LEU	Α	227	23.335		26.186	1.00 3			Č
MOTA	1720		LEU			21.389		27.590	1.00 3			Č
MOTA	1721	N			228	24.760		31.170	1.00 2			N
MOTA	1722	CA			228	25.034		32.596	1.00 2			C
MOTA	1723	С			228	25.051		33.504	1.00 2			c
MOTA	1724	0			228	24.253		34.483	1.00 2			Ö
MOTA	1725	CB			228	24.026		33.157	1.00 2			C
ATOM	1726	CG			228	24.019		32.464	1.00 2			C
MOTA	1727		TYR			24.839		32.881	1.00 2			C
ATOM	1728		TYR			23.177		31.389	1.00 2			C
									2			_

MOTA	1729	CE1 TYR			4.826		32.248	1.00 27.44
ATOM	1730	CE2 TYR	A 228		3.160	•	30.745	1.00 27.63
ATOM	1731	CZ TYR	A 228	2	3.964	48.040	31.186	1.00 29.01
ATOM	1732	OH TYR	R A 228	2	3.924	49.260	30.536	1.00 28.98
ATOM	1733		A 229	2	6.009	41.101	33.261	1.00 28.11
ATOM	1734		A 229	2	6.146	39.900	34.082	1.00 28.54
ATOM	1735		A 229		6.424	40.223	35.534	1.00 27.88
ATOM	1736		A 229		7.085	41.212	35.786	1.00 28.01
MOTA	1737		A 229		7.396	39.214	33.494	1.00 28.67
MOTA	1738		D A 229		8.116	40.314	32.802	1.00 28.96
	1739		D A 229		7.046	41.191	32.231	1.00 28.25
ATOM			R A 230		25.981	39.372	36.453	1.00 26.80
ATOM	1740		R A 230		26.296	39.542	37.840	1.00 25.91
ATOM	1741				27.838	39.508	38.028	1.00 25.72
ATOM	1742		R A 230			39.094	37.167	1.00 25.72
MOTA	1743		R A 230		28.582			1.00 25.75
MOTA	1744		R A 230		25.673	38.431	38.677	1.00 23.13
ATOM	1745		R A 230		24.193	38.523	38.900	
ATOM	1746		R A 230		23.289	38.036	37.933	1.00 24.25
MOTA	1747		R A 230			39.063	40.090	1.00 25:16
MOTA	1748		R A 230		21.944	38.105	38.139	1.00 24.40
MOTA	1749	CE2 TY	R A 230		22.311	39.114	40.320	1.00 23.86
MOTA	1750	CZ TY	R A 230	:	21.464	38.647	.39.336	1.00 26.74
ATOM	1751	OH TY	R A 230		20.122	38.713	39.501	1.00 34.04
ATOM	1752	N PR	O A 231		28.309	39.966	39.167	1.00 25.05
MOTA	1753	CA PR	O A 231		29.711	39.806	39.517	1.00 24.73
ATOM	1754		O A 231		30.151	38.318	39.500	1.00 24.94
MOTA			RO A 231		29.359	37.410	39.817	1.00 24.30
ATOM	1756		RO A 231		29.760	40.353	40.957	1.00 25.28
ATOM	1757		RO A 231		28.613	41.331	41.016	1.00 25.28
ATOM	1758		RO A 231		27.535	40.687	40.198	1.00 24.73
ATOM	1759		AL A 232		31.419	38.086		1.00 23.75
ATOM	1760		AL, A 232		31.898	36.766	39.055	1.00 24.45
ATOM	1761		AL A 232		31.725	35.935	40.351	1.00 24.83
ATOM	1762		AL A 232		31.402	34.754	40.263	1.00 24.83
ATOM	1762		AL A 232		33.375	36.761	38.582	1.00 25.13
MOTA	1764		AL A 232		33.974	35.405	38.828	1.00 23.91
			AL A 232		33.481		37.092	1.00 23.86
MOTA	1765		IS A 233		31.886			1.00 25.24
ATOM	1766				31.766			
ATOM	1767		IS A 233		30.321			
MOTA	1768		IS A 233		30.052		44.289	1.00 26.08
ATOM	1769		IS A 233					1.00 26.65
MOTA	1770		IS A 233		32.617			1.00 28.51
ATOM	1771		IS A 233		34.078		43.564	
MOTA	1772		IS A 233		34.764			
MOTA	1773		IS A 233		34.987			
MOTA	1774		IS A 233		36.043			
MOTA	1779		IS A 233		36.201			
MOTA	177		IS A 234		29.391			
MOTA	177		IS A 234		27.999			•
MOTA	177		IIS A 234		27.456			
MOTA	177		IIS A 234		27.871			
MOTA	178		IIS A 234		27.219			
MOTA	178		HIS A 234		25:782			
MOTA	178	2 ND1 H	HIS A 234		24.840			
ATOM			HIS A 234		25.105			
ATOM			HIS A 234		23.644			
MOTA			HIS A 234		23.781			
ATOM			PRO A 235		26.561	34.197	43.130	
MOTA			PRO A 235		26.018		42.678	
ATOM			PRO A 235		25.437		41.294	1.00 28.34
MOTA			PRO A 235		25.387	7 31.884	40.716	1.00 28.04
	•							

ATOM	1790	CB	PRO	A	235		24.931	32.636	43.713	1.00	29.59	С
MOTA	1791	CG	PRO				25.473	33.290	44.975		29.10	Č
MOTA	1792	CD	PRO				26.059	34.571	44.466	1.00	28.17	С
MOTA	1793	N	CYS				25.021	34.112	40.770		27.29	N
ATOM	1794	CA	CYS			•	24.447	34.135	39.455		26.15	С
ATOM	1795	С	CYS				25.478	34.602	38.451		25.39	С
MOTA	1796	0	CYS				25.140	35.102	37.361		26.21	0
ATOM ATOM	1797	CB	CYS				23.158	34.923	39.436		26.36	С
ATOM	1798 1799	SG N	CYS ASP				21.908	34.207	40.555		29.77	S
ATOM	1800	CA	ASP				26.746	34.411	38.803		24.07	· N
ATOM	1801	C	ASP				27.830 27.441	34.528 33.977	37.855		24.53	C
MOTA	1802	ŏ	ASP				26.966	32.865	36.467 36.344		24.31 23.00	C
ATOM	1803	CB	ASP				29.018	33.769	38.353		24.42	0
ATOM	1804	CG	ASP				30.233	33.850	37.414		28.30	C
MOTA	1805		ASP				30.433	34.877	36.673		29.51	0
ATOM	1806		ASP				31.071	32.900	37.386		29.51	o
MOTA	1807	N	ARG				27.633	34.803	35.445		24.85	N
MOTA	1808	CA	ARG	Α	238		27.388	34.434	34.041		26.59	Ċ
ATOM	1809	С	ARG				25.921	34.663	33.595		25.95	Č
ATOM	1810	0	ARG				25.647	34.628	32.426		26.55	0
ATOM	1811	CB	ARG			•	27.834	.32.994	33.737	1.00	26.57	С
ATOM	1812	CG	ARG				29.311	32 [.] .758	33.891		27.77	С
ATOM	1813	CD	ARG				29.727	31.360	33.399		28.78	С
ATOM	1814	NE	ARG				29.142	30.434	34.337		33.68	N
ATOM	1815	CZ			238		28.046	29.736	34.140		36.98	С
ATOM ATOM	1816 1817		ARG				27.383	29.782	32.980		38.06	N
ATOM	1818		ARG				27.609	28.987	35.129		37.87	N
ATOM	1819	N CA			239		25.012	34.933	34.516		25.97	N
ATOM	1820	CA			239		23.634 23.478	35.245	34.152		26.05	C
ATOM	1821	Ö			239		24.196	36.776 37.531	34.037		26.67	C
ATOM	1822	СВ			239		22.663	34.724	34.699 35.201		27.33 25.55	0
ATOM	1823	CG			239		23.027	33.417	35.843		27.73	C C
ATOM	1824	CD			239		23.246	32.282	34.859		31.42	c
ATOM	1825	OE1	GLN				22.332	31.881	34.133		34.43	ő
ATOM	1826		GLN				24.457	31.761	34.835		31.35	N
MOTA	1827	N	SER	Α	240		22.569	37.233	33.185		26.94	N
MOTA	1828	CA	SER	A	240		22.293	38.653	33.034		26.93	C
MOTA	1829	С	SER	Α	240		21.490	39.118	34.229		26.78	С
ATOM	1830	0			240		20.642	38.389	34.703	1.00	27.00	0
MOTA	1831	СВ			240		21.414	38.891	31.818	1.00	26.95	С
ATOM	1832	OG			240		20.916	40.234	31.804	1.00	27.75	0
ATOM	1833	N			241		21.733	40.331	34.696		26.90	N
ATOM ATOM	1834	CA			241		20.963	40.903	35.816		27.25	С
ATOM	1835 1836	C			241		19.632	41.520	35.311		27.84	C
ATOM	1837	O CB			241		18.763	41.866	36.104		27.28	0
ATOM	1838	CG			241		21.734 22.971	42.009 41.636	36.546		26.21	C
ATOM	1839	CD			241		23.740	42.877	37.344 37.817		26.53 26.65	C
ATOM	1840		GLN				23.436	43.425	38.859		31.02	c 0
MOTA	1841		GLN				24.714	43.318	37.048		28.00	. N
ATOM	1842	N			242		19.464	41.657	34.004		28.19	. N
MOTA	1843	CA			242		18.284	42.335	33.552		28.55	C
ATOM	1844 [.]	C			242		17.117	41.409	33.563		28.88	C
MOTA	1845	0			242		17.198	40.314	33.053		28.92	Ö
MOTA	1846	CB			242		18.422	42.770	32.093		29.31	Ç
MOTA	1847		VAL				17.165	43.549	31.647		27.90	· c
MOTA	1848		VAL				19.711	43.530	31.866		28.67	C
ATOM	1849	N			243		16.009	41.862	34.113		28.55	N
MOTA	1850	CA	ASP	A	243		14.766	41.103	34.052	1.00	27.62	С

ATOM	1851	С	ASP .	A	243	14.121	41.396	32.709	1.00	27.45		С
ATOM	1852	0	ASP	Α	243	13.579	42.480	32.452	1.00	25.90		0
ATOM	.1853	CB	ASP	Α	243	13.876	41.560	35.193	1.00	27.99		С
MOTA	1854	CG	ASP	A	243	12.509	40.945	35.177	1.00	29.40		C ·
ATOM	1855	OD1	ASP	A	243	12.096	40.291	34.179	1.00	31.46		0
MOTA	1856	OD2	ASP	Α	243	11.747	41.110	36.161	1.00	32.65		0
MOTA	1857	N	PHE	Α	244	14.180	40.419	31.825		28.27		N
ATOM	1858	CA	PHE	Α	244	13.656	40.603	30.496		28.92		С
MOTA	1859	С	PHE	Α	244	12.172	40.975	30.481		30.32	•	С
ATOM	1860	0	PHE	Α	244	11.728	41.643	29.561	1.00	31.01		0
ATOM	1861	CB	PHE	Α	244	13.900	39.369	29.657		29.32		С
MOTA	1862	CG	PHE	Α	244	15.255	39.298	29.053	1.00	28.51		С
ATOM	1863	CD1	PHE	Α	244	16.397	39.628	29.775		31.29		С
MOTA	1864	CD2	PHE	Α	244	15.399	38.853	27.793	1.00	28.23		С
ATOM	1865	CE1	PHE	A	244	17.649	39.535	29.196	1.00	29.39		С
ATOM	1866	CE2	PHE	Α	244	16.654	38.736	27.229	1.00	30.79		C
ATOM	1867	CZ	PHE	Α	244	17.759	39.107	27.919		29.44		С
MOTA	1868	N	ASP	A	245	11.401	40.551	31.482	1.00	31.22		N
MOTA	1869	CA	ASP	A	245	10.007	40.913	31.544	1.00	31.40		С
MOTA	1870	С	ASP	Α	245	9.770	42.349	32.032	1.00	31.91		С
ATOM	1871	0	ASP			8.704	42.891	31.786		30.40		0
MOTA	1872	CB	ASP	Α	245	9.263	39.968	32.467	1.00	32.57		С
ATOM	1873	CG	ASP	Α	245	9.292	38.546	31.988	1.00	33.29		С
MOTA	1874	OD1	ASP	A	245	9.289	38.333	30.768	1.00	35.51		0
MOTA	1875	OD2	ASP	Α	245	9.348	37.577	32.764	1.00	35.50		Ο.
ATOM	1876	N	ASN	Α	246	10.735	42.954	32.731	1.00	32.07		N.
ATOM	1877	CA	ASN	Α	246	10.562	44.310	33.244	1.00	33.10		C
MOTA	1878	·C	ASN	Α	246	11.884	45.016	33.384	1.00	32.49		С
MOTA	1879	0	ASN	Α	246	12.400	45.179	34.476	1.00	33.20		0
MOTA	1880	CB	ASN	A:	246	9.873	44.296	34.603	1.00	33.31		С
ATOM	1881	CG	ASN	Α	246	9.555	45.716	35.110	1.00	39.27		C
MOTA	1882	OD1	ASN	Α	246	9.331	46.678	34.313	1.00	43.28		0
ATOM	1883	ND2	ASN	Α	246	9.551	.45.867	36.445	1.00	44.32		N
MOTA	1884	N	PRO	Α	247	12.472	45.374	32.265	1.00	31.66		N
ATOM ·	1885	CA	PRO	Α	247	13.822	45.936	32.263	1.00	31.26		С
ATOM	1886	С	PRO	Α	247	13.924	47.298	32.933	1.00	31.58	•	С
MOTA	1887	0	PRO	Α	247	13.185	48.211	32.629	1.00	31.85		0
ATOM	1888	CB	PRO	Α	247	14.161	46:082	30.782	1.00	31.22		С
ATOM	1889	CG	PRO	Ą	247	13.017	45.510	30.022	1.00	31.05		С
MOTA	1890	CD			247	11.894	45.216	30.928	1.00	31.01		С
MOTA	1891	N			248	14.893	47.422	33.815		31.35		N
MOTA	1892	CA			248		48.643	34.467		31.48		С
MOTA	1893	С			248	16.222	49.413	33.650		31.23		С
ATOM	1894	0			248	17.422	49.217	33.784		30.76		0
ATOM	1895	CB			248	15.646	48.310	35.850		31.60		C
MOTA	1896	CG			248	15.745	49.504	36.720		33.62		C
MOTA	1897		. ASP			16.020	50.619	36.201		34.39		0
ATOM	1898				248		49.395	37.949		38.39		Ó
MOTA	1899				249	15.764	50.285	32.783		31.95		N
MOTA	1900				249	16.676	51.053	31.942		32.80		С
MOTA	1901				249	17.534	52.052	32.714		33.92		C,
MOTA	1902				249	18.558	52.490	32.203		34.33		0
ATOM	1903				249	15.906	51.732	30.825		32.56		С
MOTA	1904				249	15.183	50.751	29.928		31.41		С
MOTA	1905	CDI	TYR	A	249	15.859	49.695	29.316		30.27		. C
ATOM	1906				249	13.845	50.868	29.704		29.24		
MOTA	1907				249	15.205	48.814	28.478		29.30		·C
ATOM	1908		YYR			13.178	49.968	28.894		29.24		С
ATOM	1909				249	13.858	48.947	28.285		29.20		С
ATOM	1910				249	13.173	48.078	27.452		29.69		0
MOTA	1911	N	GŢſ	A	250	17.155	52.369	33.952	1.00	34.69		N

ATOM	1912	CA	GLU	Α	250	17.994	53.202	34.789	1.00 3	35.66		С
MOTA	1913	С	GLU	A	250	19.249	52.494	35.235	1.00			Ċ
ATOM	1914	0	GLU	A	250	20.313	53.077	35.207	1.00			0
MOTA	1915	CB	GLU			17.252	53.685	36.021	1.00	36.82		С
MOTA	1916	CG	GLU			16.115	54.609	35.650	1.00	41.99		C
ATOM	1917	CD	GLU			15.554	55.360	36.827	1.00	48.02		С
MOTA	1918		GLU			16.114	55.275	37.949	1.00 9	53.95		0
MOTA	1919	OE2	GLU	Α	250	14.543	56.043	36.614	1.00 9	52.47		0
ATOM	1920	N	ARG			19.139	51.254	35.691	1.00	33.87		N
MOTA	1921	CA	ARG			20.335	50.550	36.088	1.00	33.26		С
MOTA	1922	С	ARG			21.013	49.992	34.873	1.00	32.36		С
MOTA	1923	0	ARG			22.210	49.914	34.849	1.00			0
ATOM	1924	CB	ARG			20.040	49.425	37.066	1.00	34.36		С
ATOM	1925	CG	ARG			19.476	49.895	38.425	1.00			C
ATOM	1926	CD	ARG			18.966	48.771	39.339	1.00			С
ATOM	1927	NE	ARG			20.052	47.860	39.733	1.00			N
ATOM	1928	CZ	ARG			19.890	46.563	39.964	1.00			С
ATOM	1929		ARG			18.696	46.006	39.843	1.00			N
MOTA	1930		ARG			20.932	45.815	40.296	1.00			N
MOTA	1931	N	PHE			20.272	49.654	33.825	1.00			N
ATOM	1932	CA	PHE			20.879	48.977	32.677	1.00			С
ATOM ·	1933	C	PHE			20.528	49.651	31.347	1.00			C
ATOM	1934	0	PHE			19.882	49.096	30.483	1.00			0
ATOM ATOM	1935 1936	CB	PHE			20.420	47.531	32.675	1.00			C
ATOM	1937	CG			252	20.405	46.864	34.050	1.00			C
ATOM	1938		PHE			21.562	46.717	34.796	1.00			C
ATOM	1939		PHE			19.238	46.317	34.554	1.00			C
ATOM	1940	CE2				21.546	46.067	36.039	1.00			C
ATOM	1940	CEZ			252	19.199	45.668	35.805	1.00			C
ATOM	1941	N			253	20.356 21.034	45.551 50.844	36.550	1.00			C
ATOM	1943	CA			253	20.607	51.662	31.155 30.022		29.72		N
ATOM	1944	C			253	20.953	50.996	28.689	1.00	28.89		C
ATOM	1945	Õ			253	20.166	51.061	27.722		28.81		0
MOTA	1946	СВ			253	21.361	52.975	30.240		28.37		C
ATOM	1947	CG			253	22.543	52.614	31.155		27.97		C
ATOM	1948	CD			253	22.136	51.463	31.942		29.24		c
ATOM	1949	N			254	22.093	50.323	28.590		29.37		N
MOTA	1950	CA			254	22.401	49.742	27.274		28.85		C
MOTA	1951	С			254	21.547	48.529	26.902		28.28		Ċ
ATOM	1952	0			254	21.663	47.970	25.794		27.47		Ö
MOTA	1953	CB	ASN	A	254.	23.874	49.407	27.122		28.84		C
MOTA	1954	CG	ASN	A	254	24.745	50.654	26.996		29.96		C
MOŢA	1955		ASN			25.622	50.882	27.834		31.21	•	0
MOTA	1956	ND2	ASN	Α	254	24.531	51.443	25.931	1.00	29.17		N
MOTA	1957	N			255	20.687	48.091	27.797	1.00	27.30		N
ATOM	1958	CA			255	19.801	47.006	27.368	1.00	27.53		С
MOTA	1959	С			255	18.844	47.512	26.283	1.00	26.80		C
MOTA	1960	0			255	18.193	46.750	25.603		27.22		0
MOTA	1961	CB			255	19.015	46.448	28.538		27.48		С
MOTA	1962	CG			255	18.282	45.250	28.198		26.63		С
MOTA	1963		PHE			18.950	44.073	27.998		29.74		С
ATOM	1964		PHE			16.935	45.288	28.039		26.29		С
ATOM	1965		PHE			18.273	42.947	27.681		29.50		С
MOTA	1966		PHE			16.261	44.192	27.692		26.21		C
MOTA	1967	CZ			255	16.917	43.012	27.518		30.10		С
ATOM	1968	N			256	18.776	48.818	26.125		26.57		N
ATOM	1969	CA			256	17.918	49.429	25.137		26.55		С
ATOM ATOM	1970	C			256	18.522	49.253	23.745		26.46		С
ATOM	1971 1972	O CB			256 256	17.881	49.560	22.771		24.39		0
111061	1314	00	GIIN	A	250	17.756	50.933	25.423	1.00	26.18	•	C

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ATOM	1973 CG	G GLN A 256	16.656	51.226	26.406	1.00 28.72	С
ATOM	1974 CI			52.636	27.028	1.00 29.64	. С
ATOM		E1 GLN A 256		53.358	27.005	1.00 32.56	0
ATOM		E2 GLN A 256		52.999	27.590	1.00 26.88	N
ATOM	1977 N			48.809	23.694	1.00 27.86	N
ATOM	1978 C			48.611	22.452	1.00 29.22	С
ATOM	1979 C		20.733	47.143	22.116	1.00 30.46	С
MOTA	1980 0		21.399	46.855	21.132	1.00 32.28	Ō
	1980 C		21.897	49.232	22.510	1.00 28.50	· c
MOTA	1981 C		21.878	50.666	22.890	1.00 29.30	Č
ATOM		D1 ASN A 257	22.329	51.025	23.989	1.00 27.33	ō
ATOM			21.382	51.523	21.982	1.00 25.68	Ŋ
MOTA		D2 ASN A 257 VAL A 258	20.200	46.213	22.900	1.00 23.00	N
MOTA	1985 N		20.432	44.791	22.623	1.00 31.51	C
ATOM		A VAL A 258		44.791	21.386	1.00 32.34	Č
ATOM	1987 C		19.674	44.766		1.00 32.39	ő
ATOM	1988 0		18.543		21.081	1.00 32.23	č
MOTA		B VAL A 258	20.050	43.937	23.841	1.00 33.12	Č
MOTA		G1 VAL A 258	18.546	43.818 42.566	23.986	1.00 32.40	c
ATOM		G2 VAL A 258	20.646		23.686	1.00 36.78	N
MOTA	1992 N		20.302	43.386			C
MOTA		A VAL A 259	19.682	42.796	19.448	1.00 32.96	· C
MOTA	1994 C		19.943	41.301	19.391	1.00 33.08	0
ATOM	1995 0		21.074	40.878	19.351	1.00 33.50	C
MOTA		CB VAL A 259	20.269	43.401	18.172	1.00 33.19.	c
MOTA		CG1 VAL A 259	19.625	42.771	16.962	1.00 34.73	
ATOM		CG2 VAL A 259	20.054	44.901	18.143	1.00 32.25	И
ATOM		N GLY A 260	18.902	40.491	19.406	1.00 33.70	
ATOM		CA GLY A 260	19.091	39.052	19.368	1.00 34.16	C
MOTA		C GLY A 260	19.036	38.327	18.014	1.00 33.92	C
MOTA		O GLY A 260	18.655	38.891	16.975	1.00 33.59	0
MOTA		N TYR A 261	19.469	37.071	18.052	1.00 33.14	N
MOTA		CA TYR A 261	19.375	36.157	16.938	1.00 33.55	C
MOTA		C TYR A 261	18.439	35.095	17.489	1.00 33.41	C
MOTA		O TYR A 261	18.700	34.542	18.561	1.00 33.67	0
MOTA		CB TYR A 261	20.715	35.508	16.657	1.00 33.81	C
MOTA		CG TYR A 261		36.416	16.061	1.00 36.80	. C
MOTA		CD1 TYR A 261	21.886	36.545	14.694	1.00 42.37.	C
ATOM		CD2 TYR A 261	22.602	37.139	16.851	1.00 38.31	C
MOTA		CE1 TYR A 261	22.823	37.378	14.139	1.00 43.02	C
MOTA		CE2 TYR A 261	23.556	37.938	16.312	1.00 40.85	C
MOTA		CZ TYR A 261	23.660	38.058	14.955	1.00 42.50	С
MOTA		OH TYR A 261	24.617	38.865	14.414	1.00 45.43	0
MOTA		N GLU A 262	17.322	34.832	16.834	1.00 32.71	N
MOTA		CA GLU A 262	16.394	33.886	17.438	1.00 32.21	C
MOTA		C GLU A 262	15.975	32.768	16.508	1.00 30.89	C
MOTA		O GLU A 262	16.180	32.819		1.00 30.63	. 0
MOTA		CB GLU A 262	15.196	34.613		1.00 32.16	C
MOTA		CG GLU A 262	13.968	34.753		1.00 30.84	C
MOTA		CD GLU A 262	12.818	35.380		1.00 31.21	C
MOTA		OE1 GLU A 262	12.761	36.612		1.00 34.58	0
MOTA		OE2 GLU A 262	11.962	34.663		1.00 29.56	0
MOTA		N THR A 263	15.447	31.746			N
MOTA		CA THR A 263	14.941	30.587			C
MOTA		C THR A 263	14.080	29.743			C
MOTA		O THR A 263	14.088	29.893			. 0
MOTA		CB THR A 263	16.093	29.746			· C
MOTA		OG1 THR A 263	15.592	28.798			0
ATOM		CG2 THR A 263	16.697				C
ATOM		N VAL A 264	13.306				N
MOTA		CA VAL A 264	12.509				C
MOTA	2033	C VAL A 264	12.925	26.576	17.022	1.00 29.10	С
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ATOM	2034	0	VAL			12.876	26.279	15.828	1.00 28.47	0
ATOM	2035	CB			264	11.025	28.126	17.252	1.00 29.23	Č
MOTA	2036	CG1				10.259	26.871	17.767	1.00 29.07	Č
MOTA	2037	CG2				10.520	29.431	17.973	1.00 28.52	С
ATOM	2038	N			265	13.401	25.763	17.954	1.00 29.56	N
ATOM	2039	CA			265	13.806	24.413	17.594	1.00 29.83	C
ATOM	2040	C			265	12.785	23.404	18.039	1.00 29.63	С
ATOM	2041	0			265	12.188	23.544	19.105	1.00 29.93	0
ATOM ATOM	2042	CB			265	15.197	24.015	18.203	1.00 29.88	С
ATOM	2043 2044	CG1	VAL VAL			16.281	24.883	17.589	1.00 32.24	С
ATOM	2044	N N			266	15.234	24.114	19.712	1.00 26.80	С
ATOM	2045	CA			266	12.642 11.770	22.371	17.226	1.00 28.96	N
MOTA	2047	C			266	12.463	21.268 19.909	17.513	1.00 28.86	C
ATOM	2048	Õ			266	13.656	19.804	17.428 17.215	1.00 28.32	C
ATOM	2049	N			267	11.696	18.852	17.581	1.00 28.58 1.00 28.06	, 0
ATOM	2050	CA			267	12.278	17.505	17.565	1.00 28.00	N
MOTA	2051	С			267	13.148	17.313	16.360	1.00 28.01	, C
ATOM	2052	0			267	12.674	17.573	15.265	1.00 28.36	0
ATOM	2053	CB			267	11.047	16.582	17.482	1.00 27.55	· c
MOTA	2054	CG	PRO	Α	267	10.000	17.278	18.220	1.00 28.05	č
ATOM	2055	CD			267	10.237	18.817	17.827	1.00 28.28	Ċ
MOTA	2056	N	GLY	Α	268	14.392	16.878	16.562	1.00 27.37	N
MOTA	2057	CA			268	15.273	16.605	15.453	1.00 25.78	C
ATOM	2058	С			268	16.231	17.726	15.175	1.00 25.51	С
ATOM	2059	0			268	17.237	17.508	14.519	1.00 26.07	0
ATOM	2060	N			269	15.957	18.928	15.653	1.00 25.79	N
ATOM	2061	CA			269	16.835	20.044	15.354	1.00 25.78	. C
ATOM ATOM	2062	C			269	17.996	20.091	16.377	1.00 26.28	С
ATOM	2063 2064	O CB			269	17.848	19.689	17.549	1.00 26.27	0
ATOM	2065	CG			269 269	16.106	21.376	15.504	1.00 26.89	С
ATOM	2066	OD1			269	14.898	21.583	14.603	1.00 25.99	C
ATOM	2067		ASP			14.745 14.065	20.966 22.495	13.562	1.00 28.50	0
ATOM	2068	N			270	19.128	20.632	14.853	1.00 29.93	0
ATOM	2069	CA			270	20.291	20.832	15.937 16.775	1.00 26.28 1.00 26.03	N
ATOM	2070	С			270	20.780	22.271	16.628	1.00 26.03	C
ATOM.	2071	0			270	21.123	22.727	15.547	1.00 25.72	0
ATOM	2072	CB			270	21.414	19.938	16.381	1.00 25.72	C
ATOM	2073		VAL	Α	270	22.675	20.325	17.113	1.00 26.27	č
ATOM	2074 -	CG2	$. \mathtt{VAL}$	A	270	21.060	18.546	16.735	1.00 25.93	Č
MOTA	2075	N			271	20.809	22.987	17.730	1.00 26.47	. N
ATOM	2076	CA			271	21.257	24.364	17.713	1.00 26.42	C
ATOM	2077	C			271	22.673	24.422	18.228	1.00 27.12	С
ATOM	2078	0			271	22.973	23.936	19.310	1.00 26.82	0
ATOM	2079	CB			271	20.372	25.235	18.570	1.00 26.20	С
ATOM	2080	CG			271	20.935	26.646	18.783	1.00 27.91	С
ATOM ATOM	2081		LEU			20.962	27.396	17.500	1.00 27.86	С
ATOM	2082 2083		LEU			20.100	27.425	19.789	1.00 29.16	С
ATOM	2084	N CA			272	23.563	24.980	17.423	1.00 27.82	N
ATOM	2085	C			272 272	24.913	25.201	17.873	1.00 27.79	С
ATOM	2086	Ö			272	24.918 24.660	26.494	18.662	1.00 26.67	C
ATOM	2087	СВ			272	25.898	27.528 25.325	18.117 16.693	1.00 27.22	0
ATOM	2088	CG			272	27.296	25.785	17.124	1.00 27.26	C
MOTA	2089		TYR			27.230	25.237	18.221	1.00 28.18 1.00 28.32	C
ATOM	2090		TYR			27.973	26.784	16.435	1.00 28.32	C
ATOM	2091		TYR			29.169	25.653	18.600	1.00 29.06	C
ATOM	2092		TYR			29.232	27.188	16.805	1.00 27.19	c
MOTA	2093	CZ			272	29.821	26.632	17.903	1.00 27.13	c
MOTA	2094	OH			272	31.081	27.026	18.322	1.00 24.66	0
										•

ATOM	2095	N	ILE	A :	273	25	5.237	2	6.418	19.9	34	1.00	26.8	7		N
ATOM	2096	CA	ILE	Α	273	25	5.381	2	7.591	20.8	10	1.00	26.8	9		С
ATOM	2097	С	ILE				6.841		7.751	21.1	.82	1.00	27.3	7		С
	2098	0	ILE				7.359		7.049	22.0		1.00				0
ATOM							4.647		7.422	22.0		1.00				C
ATOM	2099	CB	ILE													
ATOM	2100		ILE				3.182		7.185	21.7		1.00				С
ATOM	2101		ILE				4.852		8.675	22.9		1.00				С
ATOM	2102	CD1	ILE	Α	273	2:	2.338	2	7.108	23.0	65	1.00	25.3	37		С
MOTA	2103	N	PRO	Α	274	2	7.491	2	8.681	20.5	15	1.00	27.3	39		N
MOTA	2104	CA	PRO			2	8.923	2	8.871	20.6	501	1.00	27.7	76		C
ATOM	2105	C	PRO				9.287		9.415	21.9		1.00			•	С
							8.483		0.135	22.5		1.00				Ö
MOTA	2106	0	PRO													C
MOTA	2107	CB	PRO				9.250		9.840	19.4		1.00				C
MOTA	2108	CG	PRO				7.980		0.107	18.		1.00				
ATOM	2109	CD	PRO	Α	274	2	6.876		9.504	19.4		1.00				С
MOTA	2110	N	MET	Α	275	3	0.467	2	9.017	22.3	394	1.00	27.	88		N
MOTA	2111	CA.	MET	Α	275	3	0.979	2	9.346	23.	717	1.00	28.	91		C
MOTA	2112	С			275		0.974		30.849	23.9	919	1.00	28.	27		С
MOTA	2113	ō			275		1.284		31.589	23.0		1.00	27.	69		0
		СВ			275		2.365		28.808	23.		1.00				C
MOTA	2114															Č
MOTA	2115	CG			275		2.861		28.842	25.		1.00				
MOTA	2116	. SD			275	_	4.499		28.084	25.			39.			S
MOTA	2117	CE	MET	Α	275	3	5.200) 2	28.479	23.			36.			С
ATOM	2118	N	TYR	Α	276	3	0.531	L 3	31.294	25.	086	1.00	27.	79		N
MOTA	2119	CA	TYR	A	276	3	30.472	2 :	32.746	25.	389	1.00	29.	16		С
ATOM	2120	C			276		9.267		33.465	24.	802	1.00	27.	80		С
ATOM	2121	ō			276		9.076		34.609	25.		1.00	28.	35		0
	2122	СВ			276		31.779		33.506	24.			29.			C
MOTA									33.207	25.			34.			č
MOTA	2123	CG			276		32.918									C
MOTA	2124	CD1			276		32.966		33.783		146		38.			
MOTA	2125	CD2	TYR	A	276	3	33.934	4	32.306		547		39.			С
MOTA	2126	CEI	LTYR	R A	276	3	33.955	5.	33.493	28.	022	1.00	39.	83		C
ATOM	2127	CE2	TYP	A S	276	3	34.965	5	32.015	26.	449	1.00	42.	05		С
MOTA	2128	CZ			276		34.954		32.609	27.	685	1.00	42.	46		С
ATOM	2129	OH			276		35.949		32.343		624		48.			0
ATOM	2130	N			277		28.468		32.830		951		27.			N
											419		26.			C
MOTA	2131	CA			277		27.27		33.485							č
MOTA	2132	С			277		26.160		33.442		424		25.			
MOTA	2133	0			277		25.882		32.409		973		26.			0
MOTA	2134	CB	TRI	? A	277	:	26.79		32.826		130		26.			С
ATOM	2135	CG	TRI	? A	277		27.52	5	33.276		957		24.			С
ATOM	2136	CD	1 TRI	P A	277		28.86	2	33.118	20.	731	1.00	24.	81		С
MOTA	2137				277		26.99		33.935		821		23.	. 88		С
MOTA	2138				277		29.20		33.674		.531		24.			N
ATOM	2139				277		28.07		34.182		944		0 24			С
ATOM	2140				277		25.72		34.398		464		0 25			Ċ
													0 23			c
ATOM	2141				277		27.92		34.858		.747					
MOTA	2142				277		25.57		35.064		.250		0 25			C
MOTA	2143				277		26.67		35.292		.414		0 24			С
MOTA	2144	N	TR	P	A 278		25.51	.6	34.566		. 673		0 26			N
MOTA	2145	CA	TR	P A	A 278		24.40	8	34.623	25	. 625	1.0	0 26	. 96		С
ATOM	2146	С			A 278		23.22		33.847		.050		0 27	.33		С
MOTA	2147				A 278		23.02		33.846		.847		0 27			0
ATOM	2148				A 278		23.95		36.062		.838		0 26			C
									36.916		.455		0 27			Ċ
MOTA	2149				A 278		24.96									Č
MOTA	2150				A 278		25.99		37.558		.833		0 28			
MOTA	2151				A 278		25.06		37.228		.830		0 25			C
MOTA	2152				A 278		26.73		38.261		.753		0 28			N
MOTA	2153		2 TR	P	A 278	•	26.16	54	38.072		.991		0, 29			С
ATOM	2154	CE	3 TR	P	A 278		24.30	3	36.915	28	.942	1.0	0 26	.86		С
ATOM	2155		22 TR	P	A 278		26.54	41	38.563	3 29	.224	1.0	0 28	.96		С

ATOM	2156	CZ3	TRP	Α	278	24.676	37.402	30.157	1.00 29.86	C
ATOM	2157	CH2	TRP	Α	278	25.780	38.224	30.293	1.00 27.89	С
MOTA	2158	N	HIS			22.455	33.193			
								25.890	1.00 27.47	Ċ Ņ
MOTA	2159	CA	HIS			21.263	32.554	25.380	1.00 28.50	С
MOTA	2160	С	HIS	Α	279	20.158	32.574	26.403	1.00 28.09	С
MOTA	2161	0	HIS	Α	279	20.420	32.445	27.584	1.00 29.26	0
ATOM	2162	СВ	HIS							
						21.528	31.112	24.899	1.00 28.46	С
MOTA	2163	CG	HIS	Ą	279	22.339	30.278	25.838	1.00 30.29	С
ATOM	2164	ND1	HIS	Α	279	23.712	30.381	25.928	1.00 31.17	N
ATOM '	2165		HIS			21.984	29.270	26.673	1.00 31.89	
ATOM	2166		HIS							C
						24.161	29.484	26.790	1.00 31.48	C
MOTA	2167	NE2	HIS			23.136	28.810	27.271	1.00 30.92	Ŋ
MOTA	2168	N	HIS	Α	280	18.942	32.764	25.916	1.00 28.12	N
ATOM	2169	CA	HIS			17.713	32.827	26.695	1.00 28.50	Ċ
ATOM	2170	C	HIS							
						16.884	31.731	26.071	1.00 28.78	С
ATOM	2171	0	HIS			16.739	31.709	24.851	1.00 29.67	0
ATOM	2172	CB	HIS	Α	280	17.069	34.196	26.498	1.00 27.71	C
MOTA	2173	CG	HIS	Α	280	15.600	34.223	26.727	1.00 29.69	Č
ATOM	2174		HIS			15.021	34.905	27.782		
									1.00 31.66	N
MOTA	2175		HIS			14.579	33.648	26.047	1.00 31.45	· C
MOTA	2176		HIS			13.710	34.743	27.738	1.00 30.66	С
MOTA	2177	NE2	HIS	·A	280	. 13.415	33.985	26.696	1.00 31.28	· N
ATOM	2178	N			281	16.346	30.814	26.860		
ATOM	2179	CA							1.00 29.23	N
					281	15.651	29.652	26.294	1.00 29.56	С
MOTA	2180	С			281	14.311	.29.497	26.922	1.00 30.16	С
ATOM	2181	0	ILE	Α	281	. 14.190	29.517	28.135	1.00 30.14	0
MOTA	2182	CB	ILE	А	281	16.478	28.409	26.516	1.00 29.69	Č
ATOM	2183		ILE							
						17.707	28.491	25.628	1.00 30.69	С
MOTA	2184		ILE			15.686	27.119	26.172	1.00 28.22	С
MOTA	2185	CD1	ILE	Α	281	18.689	27.534	25.980	1.00 33.11	C
MOTA	2186	N	GLU	Α	282	13.280	29.380	26.103	1.00 31.22	N
ATOM	2187	CA			282	11.931	29.278			
								26.665	1.00 31.99	С
MOTA	2188	C			282	11.123	28.182	26.007	1.00 31.79	С
ATOM	2189.	0			282	11.131	28.021	24.806	1.00 32.77	0
MOTA	2190	CB	GLU	Α	282	11.200	30.638	26.618	1.00 32.16	С
ATOM	2191	CG			282	11.017	31.265	25.253	1.00 33.49	· c
ATOM	2192	CD			282					
						10.378	32.663	25.313	1.00 36.22	С
MOTA	2193		GLU			10.879	33.552	26.043	1.00 38.20	0
ATOM	2194	OE2	GLÜ	Α	282	9.380	32.898	24.603	1.00 38.15	0
ATOM	2195	N	SER	Α	283	10.454	27.392	26.827	1.00 31.81	N
ATOM	2196	CA			283	9.592	26.333			
ATOM								26.331	1.00 30.79	. С
	2197	С			283	8.245			1.00 30.98	С
MOTA	2198	0	SER	Α	283	7.635	27.640	26.780	1.00 30.36	0
MOTA	2199	CB	SER	A	283	9.430	25.305	27.424	1.00 30.62	С
ATOM	2200	OG			283	10.586	24.463	27.496	1.00 29.45	
ATOM	2201	N			284					. 0
						7.776	26.790	24.709	1.00 31.06	N
MOTA	2202	CA			284	6.587	27.504	24.270	1.00 31.43	C
ATOM	2203	С	LEU	Α	284	5.398	27.390	25.204	1.00 31.82	С
MOTA	2204	0	LEU	Α	284	5.137	26.333	25.776	1.00 31.15	Ō
ATOM	2205	СВ			284	6.156	27.098			
ATOM	220.6							22.895	1.00 31.75	С
		CG			284	7.223	27.187	21.829	1.00 33.11	С
ATOM	2207		LEU			6.571	27.388	20.478	1.00 33.62	С
ATOM	2208	CD2	LEU	A	284	8.170	28.270	22.142	1.00 32.91	C
ATOM	2209	N			285	4.701	28.512	25.355		
ATOM	2210								1.00 32.74	N
		CA			285	3.481	28.564	26.147	1.00 34.35	C
MOTA	2211	С			285	2.502	27.591	25.540	1.00 34.74	С
MOTA	2212	0	LEU	A	285	2.375	27.510	24.332	1.00 34.70	0
ATOM	2213	CB			285	2.863	29.946	26.094	1.00 34.70	
ATOM	2214	CG			285					C
						3.729	31.060	26.638	1.00 34.74	С
ATOM	2215		LEU			3.183	32.369	26.160	1.00 34.14	С
MOTA	2216	CD2	LEU	A	285	3.780	30.970	28.136	1.00 34.97	С
									·	_

ATOM	2217	N	ASN A	A :	286	1.838	26.829	26.380	1.00	35.89	1	N
ATOM	2218	CA	ASN A	Δ :	286	0.841	25.863	25.896	1.00	37.12		С
			ASN A			1.363	24.809	24.909		36.14		c
MOTA	2219											
MOTA	2220	0	ASN 2			0.600	24.306	24.108		35.85		0
MOTA	2221	CB	ASN A	A :	286	-0.336 .	26.635	25.274	1.00	37.80		С
MOTA	2222	CG	ASN 2	Δ .	286	-0.882	27.690	26.219	1.00	42.02	•	С
	2223		ASN .			-1.326	27.365	27.326		47.86		ō
MOTA												-
MOTA	2224		ASN .			-0.809	28.965	25.817		46.67	•	
ATOM	2225	N	GLY .	Α	287	2.653	24.478	24.974	1.00	35.43		N
ATOM	2226	CA	GLY .	Α	287	. 3.262	23.539	24.057	1.00	34.11		С
ATOM	2227	C	GLY			3.569	22.202	24.666		34.02		С
												ō
MOTA	2228	0	GLY .			4.073	21.317	23.977		34.98		
ATOM	2229	N	GLY	A	288	3.242	22.023	25.944	1.00	33.71		N
ATOM	2230	CA	GLY	Α	288	3.476	20.759	26.616	1.00	33.00		С
ATOM	2231	С	GLY	A	288	4.908	20.692	27.107	1.00	33.19		С
ATOM	2232	Ö	GLY			5.625	21.681	26.989		33.40		0
MOTA	2233	N	ILE			5.337	19.540	27.621		32.87		N
MOTA	2234	CA	ILE	Α	289	6.647	19.425	28.195	1.00	33.57		С
ATOM	2235	С	ILE	Α	289	7.695	19.434	.27.118	1.00	33.13		C
ATOM	2236	ο.	ILE			7.454	19.023	25.995		34.41		0
										34.25		Ċ
MOTA	2237	СВ	ILE			6.809	18.137	29.006				
MOTA	2238	CG1				6.789	16.920	28.102		36.60		С
MOTA	2239	CG2	ILE	Α	289	5.746	18.005	30.113	1.00	34.91		С
MOTA	2240	CD1	ILE	Α	289	7.271	15.659	28.834	1.00	38.16		С
ATOM	2241	N	THR			8.891	19.868	27.465		31.68		N.
										29.79	•	C
ATOM	2242	CA	THR			9.956	19.853	26.498				
MOTA	2243	С	THR			11.054	18.938	26.958		27.97		С
MOTA	2244	0	THR	A	290	11.256	18.739	28.133	1.00	26.58		0
MOTA	2245	CB	THR			10.526	21.278	26.305	1.00	30.77		С
MOTA	2246	OG1				10.957	21.827	27.554		27.89		0
MOTA	2247	CG2				9.458	22.243	25.789		30.82		С
ATOM	2248	N	ILE	Α	291	11.787	18.395	26.021	1.00	26.96		N
MOTA	2249	CA	ILE	Α	291	12.910	17.594	26.383	1.00	27.83		C
ATOM	2250	С	ILE			14.059	17.952	25.493	1.00	27.31		С
ATOM	2251	Ö			291	13.880	18.028	24.289		27.83		ō
MOTA	2252	CB			291	12.596	16.104	26.195		28.72		С
MOTA	2253	CG1	ILE	Α	291	11.480	15.671	27.140	1.00	29.09		С
ATOM	2254	CG2	ILE	Α	291	13.865	15.278	26.438	1.00	28.55		C
MOTA	2255	CD1	ILE	Α	291	11.115	14.232	26.986	1.00	30.86		C
MOTA	2256	N·.			292	15.240	18.093	26.074		26.63		N
MOTA	2257	CA			292	16.415	18.444	25.333		26.88		С
MOTA	2258	С	THR	Α	292	17.587	17.724	25.915				С
ATOM	2259	0	THR	Α	292	17.631	17.524	27.102	1.00	26.40		0
ATOM	2260	CB	THR	Α	292	16.753	19.971	25.532	1.00	27.41		С
ATOM	2261	OG1			292	15.652	20.841	.25.187		28.64		0
								24.592				C
MOTA	2262		2 THR			17.852	20.398			28.03		
MOTA	2263	N			293	18.577	17.414		1.00	26.32		N
ATOM	2264	CA	VAL	Α	293	19.834	16.896	25.585	1.00	26.86		С
ATOM	2265	С	VAL	Α	293	20.964	17.718	24.978		27.24		С
MOTA	2266	Ö			293	21.011	17.892			26.60		0
ATOM	2267	CB			293	20.029	15.422	25.226		27.56		С
ATOM	2268		l VAL			21.472	15.004	25.411		27.42		С
ATOM	2269	CG2	Z VAL	Α	293	19.138	14.546	26.126	1.00	29.64		C
MOTA	2270				294	21.849	18.278	25.814		27.26		N
	2271				294	22.960	19.055	25.258		27.20		C
ATOM												
ATOM	2272				294	24.253	18.268			27.79		С
MOTA	2273	0	ASN	Α	294	24.338	17.177	25.883	1.00	28.63		0
ATOM	2274	CB			294	23.118	20.446	25.881	1.00	27.69		С
ATOM	2275				294	23.703				30.08		С
						24.309						ō
ATOM	2276		1 ASN							29.80		
ATOM	2277	ND:	2 ASN	A	294	23.513	21.506	28.064	T.00	28.15		N
										•		

ATOM	2278	N	PHE.	A	295	25.235	18.816	24.576	1.00 27.46	N
MOTA	2279		PHE .			26.548	18.219	24.428	1.00 27.53	С
MOTA	2280	С	PHE .	Α	295	27.543	19.352	24.675	1.00 28.01	С
ATOM	2281	0	PHE .	Α	295	27.720	20.239	23.811	1.00 28.48	0
MOTA	2282	CB	PHE .	A	295	26.756	17.703	23.009	1.00 27.33	С
ATOM	2283	CG	PHE .	Α	295	25.955	16.487	22.658	1.00 27.87	С
MOTA	2284	CD1	PHE	Α	295	24.586	16.560	22.496	1.00 27.75	С
MOTA	2285		PHE			26.581	15.287	22.426	1.00 26.57	C
ATOM	2286	CE1	PHE	Α	295	23.892	15.466	22.147	1.00 28.45	С
MOTA	2287	CE2	PHE	A	295	25.869	14.187	22.095	1.00 27.40	С
MOTA	2288	CZ	PHE	Α	295	24.541	14.262	21.952	1.00 27.57	С
MOTA	2289	N	TRP -			28.166	19.346	25.852	1.00 28.46	Ŋ
MOTA	2290	CA	TRP	Α	296	29.097	20.402	26.249	1.00 29.05	С
MOTA	2291	С	TRP			30.545	19.950	26.077	1.00 29.39	C
MOTA	2292	0	TRP			30.981	18.942	26.663	1.00 29.90	0
MOTA	2293	CB	TRP			28.850	20.825	27.696	1.00 29.23	C
ATOM	2294	CG	TRP			27.917	·21.982	27.908	1.00 31.21	С
ATOM	2295	·CD1	TRP			27.805	23.080	27.135	1.00 33.45	С
MOTA	2296	CD2	TRP			26.995	22.171	28.996	1.00 33.70	C
ATOM	2297	NE1	TRP			26.864	23.941	27.651	1.00 33.91	N
MOTA	2298	CE2	TRP			26.344	23.403	28.787	1.00 33.49	C
MOTA	2299		TRP			26.638	21.414	30.113	1.00 36.30	C
MOTA	2300		TRP			25.377	23.902	29.642	1.00 35.59	c
ATOM	2301	CZ3	TRP			25.643	21.899	30.967	1.00 37.80	С
ATOM	2302	CH2	TRP	Α	296	25.034	23.141	30.727	1.00 37.39	C
ATOM	2303	N	TYR			31.288	20.720	25.292	1.00 29.87	N.
MOTA	2304	CA	TYR			32.693	20.472	25.017	1.00 30.43	Ċ
MOTA	2305	С	TYR			33.548	21.629	25.518	1.00 30.98	С
MOTA	2306	0			297	33.167	22.765	25.387	1.00 29.50	0
MOTA	2307	CB			297	32.909	20.334	23.502	1.00 30.36	. C
ATOM	2308	CG			297	32.304	19.083	22,919	1.00 30.07	C
MOTA	2309	CD1			297	30.946	19.012	22.627	1.00 29.74	С
MOTA	2310	CD2	TYR			33.083	17.960	22.687	1.00 28.56	С
MOTA	2311	CE1	TYR	Α	297	30.397	17.859	22.105	1.00 28.46	С
MOTA	2312	CE2	TYR	Α	297	32.546	16.800	22.213	1.00 27.77	С
ATOM	2313	CZ	TYR	Α	297	31.202	16.758	21.913		С
ATOM	2314	OH	TYR	Α	297	30.654	15.613	21.438	1.00 27.72	0
ATOM	2315	N	LYS	Α	298	34.723	21.325	26.060	1.00 32.77	N
ATOM	2316	CA	LYS	Α	298	35.671	22.349	26.470	1.00 34.43	С
MOTA	2317	С	LYS	Α	298	36.126	23.014	25.216	1.00 34.91	С
MOTA	2318	0	LYS	Α	298	36.236	22.373	24.194.	1.00 35.28	0
MOTA	·2319	CB	LYS	A	298	36.865	21.749	27.221	1.00 35.25	. C
MOTA	2320	CG	LYS	Α	298	36.595	21.446	28.725	1.00 38.48	С
MOTA	2321	CD	LYS	Α	298	37.834	20.990	29.532	1.00 42.40	С
MOTA	2322	CE.	LYS	A	298	37.429	20.600	30.991	1.00 45.34	C
MOTA	2323	NZ	LYS	A	298	38.515	19.883	31.770	1.00 49.07	N
MOTA	2324	N	GLY	A	299	36.384	24.305	25.267	1.00 36.67	N
MOTA	2325	CA	GLY	Α	299	. 36.837	24.998	24.080	1.00 38.01	С
MOTA	2326	С	GLY	A	. 299	38.249	24.618	23.689	1.00 39.33	С
MOTA	2327	0	GLY	Α	299	38.965	23.987	24.437	1.00 39.19	0
MOTA	2328	N	ALA	Α	300	38.644	25.017	22.498	1.00 41.68	N
ATOM	2329	CA	ALA	A	300	40.014	24.844	22.048	1.00 43.93	С
ATOM	2330	С	ALA	A	300	40.964	25.618	22.940	1.00 45.88	С
ATOM	2331	0			300	40.558	26.437	23.741	1.00 46.12	0
ATOM	2332	CB	ALA	A	300	40.148	25.343	20.639	1.00 43.86	С
MOTA	2333	N			301	42.254	25.393	22.773	1.00 49.19	N
MOTA	2334	CA	PRO	A	301	43.251	26.084	23.605	1.00 50.79	С
MOTA	2335	C			301	43.465	27.525	23.204	1.00 52.01	. с
ATOM	2336	0			301	43.302	27.869	22.041	1.00 52.73	0
ATOM	2337	CB			301	44.534	25.325	23.303	1.00 50.51	C
MOTA	2338	CG	PRO	A	301	44.357	24.908	21.884	1.00 50.75	С

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7	MOTA	2339	CD	PRO A	A 3	301	42.	890	24.	521	21.766	1	.00	49.57		С
	MOTA	2340	N	THR A				.831	28.	346	24.169			53.76		N
	MOTA	2341	CA	THR A				.173	29.		23.928			55.20		С
				THR A				. 563	29.		23.307			56.14		č
	MOTA	2342	C						29.		23.980			56.50		ŏ
	MOTA	2343	0	THR A				.504								
	MOTA	2344	CB	THR A				.249		449	25.274			55.30		. С
ž	MOTA	2345	OG1					.959		448	25.909			57.92		0
1	MOTA	2346	CG2	THR .	A :	302	44	.552	31.	886	25.090			56.33		C
- 3	MOTA	2347	N	PRO .	A :	303	45	.743	30.	239	22.086	5 1	.00	56.60		Ŋ
	MOTA	2348	CA	PRO .	A :	303	47	.057	30.	145	21.427	7 1	.00	56.45		С
	ATOM	2349	С	PRO .				.168	30.	743	22.280) 1	.00	56.31		С
	ATOM	2350	Ō	PRO .				.845		449	23.235		.00	56.29		0
	ATOM	2351	CB	PRO				.883		989	20.168			56.55		С
	MOTA	2352	CG	PRO				.418		007	19.927			56.34		C
	ATOM	2353	CD	PRO				.812		082	21.309			56.48		Č
										001	18.664			61.01		N
	ATOM	2354	N	GLU				.896								C
	MOTA	2355		GLU				.873		991	17.591			61.50		c
	ATOM	2356	С	GLU				.852		079	17.834			60.73		
	MOTA	2357	0	GLU				.755		828	18.308			61.45		.0
	MOTA	2358	CB	GLU	Α	307		.614		356	16.205			62.21		С
	MOTA	2359	CG	${\tt GLU}$	Α	307	46	.871	38.	. 339	15.045	5 3	1.00	63.86		. C
	MOTA	2360	CD	GLÜ	A	307	46	.898	37.	697	.13.66	5 1	1.00	65.26		С
	MOTA	2361	OE1	GLU			46	.468	36.	. 535	13.510	6 3	1.00	65.73		0
	ATOM	2362		GLU			47	.342		. 382	12.71	8 :	1.00	67.94		0
	ATOM	2363	N	TYR				.237		.302	17.51		1.00	59.88		. N
	ATOM	2364	CA	TYR				.349		.441	17.63			59.19		С
	ATOM	2365	C	TYR				.706		. 622	16.27			58.70		С
	ATOM	2366	Ö	TYR				.224		.120	15.27			59.29		. 0
		2367				308		5.133		.665	18.09			59.18		Č
	MOTA		CB											59.73		C
	ATOM	2368	CG			308		6.677		.418	19.47					Č
	MOTA	2369		TYR				.904		.708	20.60			59.74		C
	MOTA	2370		TYR				7.912		.801	19.66			59.94		C
	MOTA	2371		TYR				5.357		.438	21.86			59.94		C C
	MOTA	2372	CE2	TYR	Α	308		3.377		.519	20.93			61.17		C
	MOTA	2373	CZ	TYR	Α	308		7.592		.843	22.03			61.68		C
	MOTA	2374	ОН	TYR	A	308	48	3.032	41	.579	23.31			63.29		0
	MOTA	2375	N	PRO	Α	309	4:	3.541	42	.258	16.23	3	1.00	57.37		N
	MOTA	2376	CA	PRO	Α	309	4:	2.849	42	.815	17.41	.1	1.00	55.72		C
	MOTA	2377	С			309	. 4:	2.113	41	.742	18.22	:5	1.00	52.85		С
	ATOM	2378	0			309		1.627		.815	17.61			53.22		0
	ATOM	2379				309		1.823		.755	16.77			56.31		С
	ATOM	2380				309				.113				57.04		С
	ATOM	2381				309		2.774		.431	14.98			57.43		Ċ
	ATOM	2382				310		1.998		.879	19.54			49.67		N
														47.23	•	C
	ATOM	2383				310		1.368		.825	20.36					C
	ATOM	2384				310		9.870		:656	20.12			45.07		
	MOTA	2385				310		9.131		. 635	19.95			45.94		0
	MOTA	2386				310		1.568		109	21.83			46.99		C
	MOTA	2387				310		2.579		.351	22.70			46.52		C
	ATOM	2388		1 LEU				3.856		0.028				45.64		С
	MOTA	2389	CD	2 LEU	I A	310	4	2.840	41	1.179	23.97	75	1.00	46.57		С
	ATOM	2390	N	LYS	A	311	3	9.408	39	.414	20.13	39	1.00	41.52		. И
	ATOM	2391	. CA	LYS	A	311		7.987		.155	20.00	03	1.00	38.55		С
	ATOM	2392				311		7.179		9.463		76	1.00	35.80		С
	ATOM	2393				311		7.664		9.425				34.43		0
	ATOM	2394				311		7.760			19.5			39.46		С
	ATOM	2395				312		5.920		786				32.82		N
	ATOM	2396				312		5.055		0.081				30.91		C
	ATOM	2397				312		5.152		9.033				30.00		č
	ATOM	2398				312		5.231		9.382				28.68		ŏ
	ATOM	2399				312		3.625		0.234				30.07		Č
	WI ON	2393	, СВ	. vm		12	3		, 31	2.3	21.7	J.		5 50.07		·

ATOM	2400	N	HIS	Α	313	35.148	37.753	22.916	1 00	29.85		N
ATOM	2401	CA	HIS			35.125	36.727	23.931		30.47		N C
ATOM	2402	С	HIS			36.410	36.710	24.689		29.99		C
ATOM	2403	Ó	HIS			36.439	36.320	25.846		29.25		
ATOM	2404	СВ	HIS			34.787	35.331	23.392		31.64		0
ATOM	2405	CG	HIS			35.860	34.714	22.566				C
ATOM	2406		HIS			35.987	34.714	21.208		35.54		С
ATOM	2407				313	36.844	33.846	22.891		41.10		N
ATCM	2408		HIS			37.047				40.77		C
ATOM	2409		HIS				34.303	20.750		40.02.		C
ATOM	2410	N			314	37.567	33.603	21.743		41.82		N
ATOM	2411	CA	GLN			37.482 38.754	37.137	24.056		29.68		N
ATOM	2412	C					37.185	24.751		29.77	•	С
ATOM	2412	0	GLN			38.729	38.294	25.817		30.57		С
ATOM	2413	CB	GLN			39.222	38.120	26.956		29.69		0
ATOM	2415		GLN			39.893	37.401	23.743		30.02		С
ATOM		CG	GLN			40.111	36.182	22.786		29.84		С
ATOM	2416	CD	GLN			41.126	36.437	21.687		31.76		С
	2417	OE1	GLN			40.982	37.377	20.885		32.81		0
ATOM	2418	NE2	GLN			42.160	35.594	21.637		34.23		N
ATOM	2419	N			315	38.111	39.421	25.471		30.44		N
ATOM	2420	CA	LYS			38.026	40.491	26.431		31.27		С
ATOM	2421	C			315	37.192	40,023	27.635		30.75		С
ATOM	2422	0			315	37.511	40.373	28.784		29.60		0
ATOM	2423	CB			315	37.461	41.752	25.808	1.00	31.76		С
MOTA	2424	CG			315	38.483	42.491	24.982		33.90		С
ATOM	2425	CD			315	37.902	43.711	24.329	1.00	37.97		С
MOTA	2426	CE			315	38.911	44.380	23.419	1.00	41.69		С
ATOM	2427	NZ			315	38.264	45.411	22.536	1.00	44.93		N
MOTA	2428	N			316	36.163	39.216	27.362	1.00	29.26		N
ATOM	2429	CA			316	35.318	38.731	28.422	1.00	29.23		С
ATOM	2430	С	VAL	Α	316	36.152	37.841	29.339	1.00	29.87		С
MOTA	2431	0			316	36.075	37.926	30.584		30.33		0
MOTA	2432	CB			316	34.079	37.973	27.900	1.00	28.68		С
MOTA	2433				316	33.306	37.376	29.037		28.32	•	C
MOTA	2434	CG2	VAL	Α	316	33.144	38.887	27.136		28.57		C
MOTA	2435	N	ALA	Α	317	36.976	37.007	28.728		29.36		N
ATOM	2436	CA	ALA	Α	317	37.878	36.136	29.487		29.26		C
ATOM	2437	С	ALA	Α	317	38.776	36.941	30.389		28.08		Č
ATOM	2438	0	ALA	Α	317	39.052	36.564	31.519		27.65		ō
ATOM	2439	CB	ALA	A	317	38.733	35.267	28.561		28.70	•	Č
MOTA	2440	N	ILE	Α	318	39.211	38.068	29.873		28.33		N
ATOM	2441	CA	ILE	Α	318	40.083	38.945	30.628		28.40		C
ATOM	2442	·C			318	39.338	39.526	31.825		28.94		c
ATOM	2443	0			318	39.880	39.503	32.924		29.70		ŏ
ATOM	2444	CB			318	40.697	40.053	29.732		27.74		č
ATOM	2445	CG1			318	41.683	39.443	28.743		28.14		c
ATOM	2446	CG2	ILE	Α	318	41.433	41.082	30.577		27.98		c
MOTA	2447		ILE			42.271	40.447	27.759		29.17		C
MOTA	2448	N			319	38.115	40.032	31.630		28.75		N
ATOM	2449	CA			319	37.402	40.666	32.735		28.64		
MOTA	2450	C			319	37.140		33.877		29.22		C
ATOM	2451	Ō			319	37.308	39.981	35.082		30.32		C
MOTA	2452	СВ			319	36.123						0
ATOM	2453	CG			319	36.327	41.355	32.273		28.33		C
ATOM	2454	SD			319	34.779	42.553	31.334		27.88		C
ATOM	2455	CE			319	34.779	43.349	30.857		29.90		S
ATOM	2456	N			320		42.288	29.455		28.71		С
ATOM	2457	CA			320	36.802	38.446	33.515		29.22		N
ATOM	2458	CA				36.543	37.429	34.520		28.75		C
ATOM	2459	0			320	37.806	37.221	35.325		28.81		C
ATOM	2460	CB			320	37.782	37.132	36.569		28.76		0
-11011	4300	CD	אמט	A	320	36.142	36.118	33.861	1.00	28.67		С

MOTA	2461	CG	ARG Z	A	320		34.810	36.125	33.120	1.00 29.62	С
ATOM	2462	CD	ARG Z	A	320		34.371	34.747	32.603	1.00 27.74	C
MOTA	2463	NE	ARG 2				34.193	33.843	33.716	1.00 24.81	N
ATOM	2464	CZ	ARG 2	A	320		33.161	33.887	34.526	1.00 27.65	C
ATOM	2465	NH1	ARG 2				32.180	34.752	34.330	1.00 29.97	N
ATOM	2466		ARG 2			•	33.088	33.064	35.542	1.00 27.59	N
ATOM	2467	N	ASN :				38.933	37.167	34.627	1.00 28.60	N
ATOM	2468	CA.	ASN.				40.185	36.884	35.320	1.00 28.16	C
ATOM	2469	C	ASN				40.526	38.003	36.291	1.00 28.13	č
ATOM	2470	Ö	ASN .				40.945	37.742	37.423	1.00 29.13	ő
ATOM	2471	CB	ASN				41.318	36.615	34.319	1.00 28.09	· c
ATOM	2472	CG	ASN .				41.317	35.177	33.817	1.00 27.94	č
ATOM	2473		ASN				40.924	34.286	34.555	1.00 27.34	Ö
ATOM	2474		ASN				41.751	34.200	32.560	1.00 23.58	N
ATOM	2475	N	ILE				40.337	39.250	35.876	1.00 23.38	N
ATOM	2476	CA	ILE				40.659	40.350	36.749	1.00 27.49	C
ATOM	2477	C	ILE								
ATOM	2478	0	ILE				39.792	40.209	38.017	1.00 27.39	C
ATOM	2479	CB	ILE				40.284	40.315	39.101	1.00 26.48	0
							40.353	41.680	36.059	1.00 28.04	C
ATOM	2480	CG1					41.302	41.941	34.897	1.00 30.79	C
ATOM	2481		ILE				40.426	42.832	37.038	1.00 28.09	C
ATOM	2482		ILE				42.756	41.766	35.226	1.00 32.31	C
ATOM	2483	N	GLU				38.494	39.961	37.854	1.00 27.37	N
ATOM	2484	CA	GLU				37.618	39.868	38.985	1.00 27.48	С
ATOM	2485	С	GLU				38.060	38.784	39.881	1.00 27.52	С
ATOM	2486	0	GLU				38.096	38.956	41.079	1.00 26.90	0
ATOM	2487	CB	GLU				36.183	39.637	38.558	1.00 27.48	C
MOTA	2488	CG	GLU				35.592	40.849	37.910	1.00 27.65	С
ATOM	2489	CD	GLU				34.199	40.631	37.318	1.00 25.69	С
MOTA,	2490		GLU				33.236	40.358	38.050	1.00 24.42	0
MOTA	2491		~GLU				34.072	40.808	36.101	1.00 24.98	0
MOTA	2492·	N	LYS				38.419	37.659	39.297	1.00 29.13	N
ATOM	2493	CA	LYS	Α	324		38.845	36.508	40.097	1.00 30.35	С
MOTA	2494	С	LYS	Α	324		40.099	36.825	40.912	1.00 31.16	С
MOTA	2495	0	LYS	Ą	324		40.123	36.547	42.111	1.00 32.01	0
MOTA	2496	CB	LYS	Α	324		39.116	35.289	39.222	1.00 30.16	· C
MOTA	2497	CG	LYS	Α	324		37.887	34.625	38.648	1.00 30.63	С
MOTA	2498	CD	LYS	Α	324		38.344	33.454	37.765	1.00 30.70	. С
MOTA	2499	CE	LYS	Α	324		37.204	32.713	37.038	1.00 30.66	С
MOTA	2500	NZ	LYS	A	324		37.728	31.451	36.325	1.00 27.19	· N
ATOM	2501	N	MET	Α	325		41.119	37.401	40.270	1.00 31.84	N
MOTA	2502	CA	MET	Α	325		42.392		40.939		С
MOTA	2503	С			325		42.216		42.078	1.00 32.44	С
MOTA	2504	0			325		42.840	38.637	43.141	1.00 30.36	Ō
MOTA	2505	CB			325		43.417	38.276	39.923	1.00 32.98	C
MOTA	2506	CG			325		43.978	37.216	39.032	1.00 36.70	C
ATOM	2507	SD			325		44.734	37.879	37.532	1.00 46.02	S
ATOM	2508	CE					45.616	39.197	38.250	1.00 46.11	c
MOTA	2509	N			326		41.376	39.738	41.837	1.00 33.01	N
ATOM	2510	CA			326		41.116	40.756	42.852	1.00 34.17	C
MOTA	2511	C			326		40.490	40.151	44.083	1.00 33.83	
ATOM .	2512	Ō			326		40.871	40.464	45.188	1.00 33.22	
ATOM	2513	СВ			326		40.185	41.818	42.305	1.00 33.22	
ATOM	2514	CG			326		40.740	43.194	41.974	1.00 37.32	
ATOM	2515		LEU				42.251	43.194	41.924	1.00 37.32	
ATOM	2516		LEU				40.158	43.607	40.643	1.00 39.32	
ATOM	2517	N			327		39.534	39.262	43.861	1.00 34.50	
ATOM	2518	CA			327		38.842	38.569	44.930	1.00 34.50	
MOTA	2519	C			327		39.796		44.930	1.00 34.87	
ATOM	2520	0			327		39.798			1.00 35.34	C
ATOM	2521	N			328	•	40.725		47.016		
AIOM	4341	r _A	GTTO	14	. 320		40.725	37.081	45.139	1.00 35.88	N

ATOM	2522	CA	GLU :	A	328	41.708	36.346	45.926	1.00 36.96	С
ATOM	2523		GLU .			42.668	37.302	46.614	1.00 35.46	č
ATOM	2524		GLU			42.958	37.144	47.799	1.00 35.65	Ö
ATOM	2525		GLU .			42.465	35.340	45.074	1.00 33.03	
ATOM	2526	CG	GLU .			41.555	34.272	44.481		C
	2527						32.905		1.00 43.40	C
ATOM		CD	GLU .			41.694		45.135	1.00 50.39	C
MOTA	2528					42.006	32.861	46.361	1.00 53.07	0
MOTA	2529		GLU			41.503	31.876	44.396	1.00 53.24	0
MOTA	2530	N	ALA			43.110	38.331	45.906	1.00 34.23	N
MOTA	2531	CA	ALA	Α	329	·44.130	39.208	46.469	1.00 33.82	С
ATOM	2532	С	ALA	Α	329	43.652	40.031	47.632	1.00 33.70	. C
ATOM	2533	0	ALA	A	329	44.384	40.279	48.547	1.00 33.79	. 0
ATOM	2534	CB	ALA	Α	329	44.711	40:079	45.428	1.00 33.36	Ċ
ATOM	2535	N	LEU			42.410	40.451	47.602	1.00 34.57	N
ATOM	2536	CA	LEU			41.869	41.243	48.694	1.00 35.04	Ċ
ATOM	2537	С	LEU			41.351	40.397	49.837	1.00 35.04	c
MOTA	2538	Ö	LEU			41.011	40.922	50.884		
ATOM	2539	CB	LEU						1.00 35.39	0
	2540	CG				40.721	42.096	48.182	1.00 34.85	C
MOTA			LEU			41.141	43.081	47.095	1.00 35.83	C
ATOM	2541.		LEU			39.907	43.564	46.304	1.00 37.05	С
MOTA	2542		LEU			41.842	44.244	47.662	1.00 34.12	С
MOTA	2543	N	GLY			41.223	39.098	49.619	1.00 36.20	N
MOTA	2544	CA	GLY			40.751	38.207	50.659	1.00 36.87	C
MOTA	2545	С	GLY	A	331	39.260	38.250	50.957	1.00 37.48	С
MOTA	2546	0	GLY	Α	331	38.807	37.527	51.846	1.00 38.53	0
ATOM	2547	N	ASN	A	332	38.509	39.085	50.242	1.00 37.67	N
ATOM	2548	CA	ASN			37.069	39.175	50.399	1.00 38.06	C
MOTA	2549	С	ASN			36.446	39.652	49.088	1.00 37.75	Č
ATOM	2550	Ō	ASN			36.688	40.760	48.661	1.00 37.42	ō
MOTA	2551	CB	ASN			36.728	40.152	51.523	1.00 37.42	
ATOM	2552	CG	ASN			35.272	40.103			C
ATOM	2553				332			51.896	1.00 40.34	C
							39.377	51.274	1.00 43.85	0
MOTA	2554		ASN			-34.894	40.841	52.937	1.00 41.75	N
MOTA	2555	N			333	35.628	38.839	48.451	1.00 37.92	N
ATOM	2556	CA			333	. 35.076	39.209	47.146	1.00 37.97	С
ATOM	2557	С			333	34.245	40.456	47.211	1.00 37.96	. С
MOTA	2558	0			333	34.086	41.143	46.204	1.00 37.81	0
ATOM	2559	CB			333	34.182	38.024	46.770	1.00 37.85	C
ATOM	2560	CG	PRO	Α	333	34.327	37.037	47.801	1.00 38.26	C
ATOM	2561	CD	PRO	Α	333	35.161	37.530	48.908	1.00 37.98	. С
MOTA	2562	N	GLN	A	334	33.702	40.741	48.381	1.00 38.23	N
ATOM	2563	CA	GLN	A	334	32.872		48.539		C
ATOM	2564	С			334	33.713	43.177	48.442	1.00 37.04	Č
ATOM	2565	Ō			334	33.185	44.254	48.276	1.00 37.42	ő
ATOM	2566	CB			334	32.041	41.870	49.850	1.00 37.42	č
ATOM	2567	CG			334	30.696	41.057	49.612	1.00 33.37	C
ATOM	2568	CD			334	29.669		50.756		
ATOM	2569						41.117		1.00 49.62	С
			GLN			29.666		51.566	1.00 53.65	0
MOTA	2570				334	28.781	40.106	50.808	1.00 50.33	N
ATOM	2571	N			335	35.026	43.036	48.489	1.00 35.15	N
MOTA	2572	CA			335	35.872	44.193	48.385	1.00 34.55	С
ATOM	2573	С			335	36.197		46.927	1.00 33.05	C
ATOM	2574	0			335	36.760		46.640	1.00 32.79	0
MOTA	2575	CB			335	37.144	44.028	49.247	1.00 35.19	С
MOTA	2576	CG	GLU	A	335	36.927	44.326	50.727	1.00 37.92	С
ATOM	2577	CD			335			51.550	1.00 43.46	Č
ATOM	2578		GLU			39.179		51.179	1.00 46.92	ō
ATOM	2579		GLU			38.211		52.589	1.00 49.17	ő
MOTA	2580	N			336	35.792		46.005	1.00 31.25	N
MOTA	2581	CA			336	36.081	43.810	44.579	1.00 31.23	C
ATOM	2582	C			336	35.505		43.957	1.00 29.91	C
		-	4 . 344	-		JJ. JUS	33.010	33.331	1.00 29.00	C

ATOM	2583 O VAL A	A 336	36.177	45.816	43.246	1.00 29.08		0
ATOM	2584 CB VAL A		35.648	42.584		1.00 30.21	•	С
MOTA	2585 CG1 VAL A		35.743	42.805	42.325	1.00 29.11	•	С
ATOM	2586 CG2 VAL A		36.540	41.391	44.161	1.00 29.98		С
ATOM	2587 N GLY		34.263	45.354	44.240	1.00 28.54		N
		A 337	33.644	46.546	43.722	1.00 27.74		C
MOTA				47.848	44.130	1.00 27.74		Ċ
MOTA		A 337	34.285		43.281	1.00 27.24		Ö
ATOM		A 337	34.599	48.687				N
MOTA		A 338	34.365	48.094	45.428	1.00 27.19		C
MOTA		A 338	34.994	49.334	45.905	1.00 26.74		c
ATOM		A 338	36.378	49.553	45.328	1.00 26.42		
MOTA		A 338	36.678	50.668	44.932	1.00 27.57		0
MOTA		A 338	35.008	49.173	47.426	1.00 25.92		C ·
ATOM		A 338	33.800	48.384	47.682	1.00 27.15		C
ATOM	2597 CD PRO	A 338	33.750	47.326	46.531	1.00 27.09		С
MOTA	2598 N LEU	A 339	37.199	48.533	45.225	1.00 25.95		N
MOTA	2599 CA LEU	A 339	38.505	48.762	44.652	1.00 26.15		C
MOTA	2600 C LEU	A 339	38.384	49.205	43.192	1.00 25.74		С
ATOM		A 339	39.021	50.203	42.784	1.00 23.97		0
ATOM		A 339	39.375	47.521	44.763	1.00 27.19		С
ATOM		A 339	40.835	47.787	44.367	1.00 28.71		С
ATOM		A 339	41.805	47.124	45.241	1.00 31.14		С
ATOM	2605 CD2 LEU		41.028	47.264	42.987	1.00 30.12		С
ATOM		A 340	37.555	48.491	42.416	1.00 25.64		N
MOTA		A 340	37.364	48.841	40.991	1.00 25.90	•	C
MOTA		A 340	36.860	50.261	40.871	1.00 26.04		Ċ
ATOM		A 340	× 37.324	51.044	40.034	1.00 25.93		Ö
		A 340	36.399	47.900	40.293	1.00 25.64		Č
ATOM				46.521	40.072	1.00 27.50		č
MOTA		A 340	36.996		39.555	1.00 26.88		Ċ
ATOM	2612 CD1 LEU		35.943	45.559				C
MOTA	2613 CD2 LEU		38.221	46.587	39.138	1.00 26.63		N
MOTA		A 341	35.914	50.610	41.720	1.00 26.45		
MOTA		A 341	35.377	51.963	41.669	1.00 27.35		C
MOTA		A 341	36.450	52.983	41.983	1.00 27.08		C
MOTA		A 341	36.578	54.012	41.324	1.00 26.82		0
MOTA		A 341	34.183	52.117	42.619	1.00 27.50	•	C
MOTA		A 341	32.901	51.709	41.975	1.00 28.85		C
ATOM	2620 OD1 ASN		32.509	52.283	40.957	1.00 37.23		0
MOTA	2621 ND2 ASN	A 341	32.263	50.697	42.504	1.00 29.29		N
ATOM	2622 N · THR	A 342	37.234	52.665	42.994	1.00 26.89		N
ATOM	2623 CA THR	A 342	38.321	53.509	43.355	1.00 27.22		С
MOTA	2624 C THR	A 342	39.301	53.629	42.191	1.00 27.16		С
MOTA		A 342	39.861	54.686	42.003	1.00 26.86		0
MOTA		A 342	38.995	52.934	44.568	1.00 27.76		. С
ATOM	2627 OG1 THR		38.212	53.248	45.734	1.00 29.14		Ο.
MOTA	2628 CG2 THR		40.367		44.784	1.00 28.62		С
ATOM		A 343	39.502			1.00 26.80		N
ATOM		A 343	40.401			1.00 27.48		C
ATOM		A 343	39.927			1.00 27.78	•	С
MOTA		A 343	40.762			1.00 26.44		0
MOTA		A 343	40.602			1.00 28.13		С
ATOM		A 343	41.758			1.00 30.19		Č
ATOM		A 343	42.279			1.00 30.13		Š
		A 343	42.279					Č
ATOM							•	Ŋ
ATOM		E A 344	38.619					C
ATOM		E A 344	38.193					C
MOTA		E A 344	37.712					o
ATOM		E A 344	37.879					
MOTA		E A 344	37.146					C
ATOM			35.766					C C
. ATOM	2643 CG2 ILI	E A 344	37.457	52.176	36.667	1.00 32.43		C

ATOM	2644	CD1	ILE	A	344	34.724	53.358	36.590	1.00	35.46	c	,
ATOM	2645	N	LYS	А	345	37.107	56.032	39.108		27.79	N	
MOTA	2646	CA	LYS			36.518	57.364	39.218		28.48	Ċ	
MOTA	2647	С	LYS			37.489	58.485	39.219	1.00	27.72	C	
ATOM	2648	0	LYS			38.428	58.555	40.000	1.00	27.37	C	
ATOM	2649	CB	LYS			35.542	57.611	40.343		29.78	C	
ATOM	2650	CG	LYS			35.537	56.758	41.491	1.00	34.49	C	
MOTA	2651	CD	LYS			34.075	56.352	41.692		37.43	C	
ATOM ATOM	2652	CE	LYS			33.508	57.036	42.904		40.47		
ATOM	2653 2654	NZ N	LYS			34.223	56.522	44.138		46.19	Ŋ	
ATOM	2655	CA			346. 346	37.218	59.386	38.297		26.82	I.	
ATOM	2656	C			346	38.044 39.314	60.538	38.108		25.95	Ç	
ATOM	2657	Ö			346	40.172	60.175 61.022	37.392 37.244		25.08	C	
ATOM	2658	N	ARG			39.419	58.935	36.944		24.91 24.84	(
ATOM	2659	CA	ARG			40.647	58.436	36.347		25.30	ŀ	N C
MOTA	2660	С	ARG			40.431	57.848	34.937		26.05		3
MOTA	2661	0	ARG			41.138	58.196	34.007		24.59		5
MOTA	2662	CB	ARG	A	347	41.279	57.395	37.272		25.27		
ATOM	2663	CG	ARG	A	347	41.716	57.934	38.696		24.21		2
MOTA	2664	CD	ARG	Α	347	43.159	57.506	39.082		25.10		2
ATOM	2665	·NE	ARG	A	347	43.175	56.084	39.017		24.49		Į.
ATOM	2666	CZ			347	44.102	55.293	38.566	1.00	19.51		2
ATOM	2667		ARG			45.299	55.692	38.195	1.00	21.86		N
MOTA	2668		ARG			43.802	54.011	38.579		18.94	. 1	N
MOTA	2669	N			348	39.438	56.991	34.794		27.91		N
ATOM ATOM	2670 2671	CA			.348	39.119	56.380	33.507		29.80		C
ATOM	2672	C O			348	37.671	56.590	33.065		32.00		C
ATOM	2673	СВ			348 348 ·	37.309	56.173	31.964		32.29		0
ATOM	2674	CG			348	39.379 40.836	54.877	33.543		28.38		C
ATOM	2675	CD1			348	41.617	54.498 54.473	33.597 32.446		27.86		
ATOM	2676	CD2			348	41.422	54.124	34.787		26.79 25.32		0
MOTA	2677	CE1			348	42.945	54.106	32.496		25.35		C
MOTA	2678	CE2			348	42.734	53.762	34.847		27.07		C
ATOM	2679	CZ	TYR	Α	348	43.507	53.759	33.700		26.40		c
MOTA	2680	OH	TYR	Α	348	44.827	53.378	33.789		22.93		0
MOTA	2681	N			349	36.824	57.193	. 33.894	1,00	34.78		N
ATOM	2682	CA			349	35.426	57.360	33.473	1.00	37.16		С
MOTA	2683	C			349	34.997	58.760	33.104		38.90		C
ATOM	2684	0			349	35.690	59.756	33.136		38.66		0
ATOM ATOM	2685 2686	CB			349	34.474	56.837	34.493		36.69		С
MOTA	2687	CG OD1			349	34.480	57.633	35.727		39.34		C
MOTA	2688		ASN ASN			35.229 33.654	58.632	35.875		40.92		0
ATOM	2689		ASN			33.854	57.188 58.954	36.684		42.73		И
TER	2690	0			349	33.034	. 30.934	32.689	1.00	44.16	(0
ATOM	2691	N			795	45.870	35.442	31.163	1 00	49.68	,	A.T
MOTA	2692	CA			795 ·	44.790	36.472	31.262		49.90		N C
ATOM	2693	С			795	43.668	36.155	30.294		50.12		C
MOTA	2694	0			795	42.492	36.182	30.666		49.41		0
MOTA	2695	CB	LEU	S	795	45.331	37.873	31.004		50.09		C
MOTA	2696	CG			795	44.774	38.924	31.976		50.19		C
MOTA	2697		LEU			44:929	38.464	33.388		50.50		C
ATOM	2698		LEU			45.436	40.280	31.876		51.23		C
ATOM	2699	N			796	44.041	35.979	29.033	1.00	50.69	1	N
MOTA	2700	CA			796	43.178	35.421	27.997		51.67	(С
ATOM	2701	C			79.6	42.734	33.983	28.241		51.11	(C
ATOM ATOM	2702 2703	O CB			796	41.884	33.464	27.535		51.41		0
ATOM	2703		THR		796 796	43.888	35.547	26.626		51.86		C
	03	231	*1117	٦	190	43.253	34.704	25.671	1.00	56.26	(0

ATOM	2705	CG2	THR S		45.272	34.981	26.662	1.00 5			С
MOTA	2706		SER S		43.261	33.330	29.248	1.00			N .
MOTA	2707		SER S		42.838	31.965	29.497	1.00			С
MOTA	2708		SER S		41.471	31.865	30.165	1.00			C.
MOTA	2709		SER S		41.070	32.733	30.934	1.00			0
MOTA	2710		SER S		43.850	31.247	30.351	1.00			C
MOTA	2711		SER S		43.687	31.623	31.697	1.00			O N
MOTA	2712		TYR S		40.783 39.424	30.761 30.584	29.904 30.372	1.00			C
MOTA	2713 2714		TYR S		39.424	29.271	31.042	1.00			C
ATOM ATOM	2715		TYR S		39.880	28.305	30.827	1.00			ŏ
ATOM	2716		TYR S		38.437	30.747	29.214	1.00			Č
ATOM	2717		TYR S		38.599	29.821	28.015	1.00			C
ATOM	2718		TYR S		39.595	30.035	27.059	1.00	62.78		С
ATOM	2719		TYR S		37.689	28.783	27.793	1.00	64.68		С
ATOM	2720		TYR S		39.708	29.207	25.943	1.00	65.08		С
ATOM	2721	CE2	TYR S		37.798	27.944	26.669	1.00	66.15		С
MOTA	2722	CZ	TYR S	5 798	38.808	28.155	25.755		65.29		С
ATOM	2723	OH	TYR S		38.902	27.335	24.652		64.08		0
MOTA	2724	N		s 799	38.117	29.240	31.843		55.66		N
MOTA	2725	CA	ASP S		37.727	28.032	32.546		55.90		C
MOTA	2726	С	ASP S		36.636	27.385	31,739		54.64		C
MOTA	2727	0		s 799	36.430	27.785	30.604		55.18	•	0 C
ATOM	2728	CB		S 799	37.212	28.367 27.225	33.948		56.52 57.36		C
MOTA	2729	CG.	ASP :		37.366	26.147	34.906 34.720		57.64		Ö
. ATOM	2730 .2731			S 799 S 799	36.749 38.108	27.331	35.881		62.28		ŏ
ATOM ATOM	2732	N		S 800	35.915	26.428	32.326		53.45		N
ATOM	2733	CA		S 800	34.887	25.693	31.594		52.63		C
ATOM	2734	C		S 800	33.564	25.644	32.359		51.79		C
ATOM	2735	ŏ		S 800	32.871	24.632	32.357		51.30		0
ATOM	2736	СВ		S 800	35.372	24.282	31.327		52.47		C .
ATOM	2737			S 800	35.703	23.408	32.872	1.00	52.72		S
MOTA	2738	N	GLU	S 801	33.187	26.742	32.996	1.00	50.91		И
MOTA	2739	CA		S 801	31.939	26.732	33.762		50.65		С
MOTA	2740	С		S 801	.30.657	26.939	32.909		50.18		C
ATOM	2741	0	GLU		30.617	27.687	31.928		48.39		0
MOTA	2742	CB	GLU		32.008	27.713	34.929		50.49		C
ATOM	2743	CG	GLU		33.199	27.450	35.853		51.78		C
ATOM	2744			S 801	33.234	28.359	37.092		51.24 49.25		0
ATOM	2745			S 801 -	32.589 33.919	28.038 29.395	38.102 37.063		51.89		o
ATOM ATOM	²⁷⁴⁶ 2747	N.		S 801 S 802	29.624	26.213			50.54		И
ATOM	2748	CA		S 802	28.338	26.161			50.71		C
MOTA	2749			S 802	27.213	26.094			51.25		С
ATOM	2750	ō		S 802	27.464	25.960			50.69		0
ATOM	2751	СВ		S 802	28.286				50.61		C
ATOM	2752	CG1		S 802·	29.420		. 30.727		49.62		С
MOTA	2753	CG2	Z VAL	S 802	28.376	23.601	32.585		49.78		С
MOTA	2754	N		S 803	25.967				52.55		N
MOTA	2755			S 803	24.816				53.28		C
MOTA	2756			S 803	24.516				54.95		C
MOTA	2757			S 803	23.440				54.22		0
MOTA	2758			S 803	23.560				53.04		C
ATOM	2759			S 803	23.546				51.60		C
ATOM	2760			S 803	24.576				51.13 46.28		И
ATOM	2761			S 803 S 804	22.367 25.498				57.29		N
MOTA MOTA	2762 2763			. S 804 . S 804	25.496				59.38		C
ATOM	2764			. S 804	26.596				61.01		Č
. ATOM	2765			S 804	27.667				61.45		ō
	2,100		1	. 5 004	2			,,			_

B.mov.	05.66			_					
ATOM	2766	CB			804	25.315	21.603	34.716	1.00 59.47
MOTA	2767	N			805	26.438	21.707	37.732	1.00 62.94
ATOM	2768	CA	PRO	S	805	27.547	21.398	38.652	1.00 63.79
MOTA	2769	С	PRO	S	805	28.616	20.498	38.003	1.00 64.48
ATOM	2770	0			805	28.368	19.875		
ATOM	2771	CB			805	26.851		36.970	1.00 65.26
ATOM	2772	CG					20.654	39.807	1.00 63.79
ATOM	2773				805	25.582	20.066	39.187	1.00 63.48
		CD			805	25.175	21.035	38.107	1.00 63.26
A?OM	2774	N			806	29.779	20.405	38.630	1.00 65.18
MOTA	2775	CA			806	30.903	19.626	38.100	1.00 65.66
ATOM	2776	С	ILE	S	806	30.853	18.145	38.489	1.00 65.84
MOTA	2777	0	ILE	S	806	30.287	17.780	39.522	1.00 66.22
ATOM	2778	CB			806	32.239	20.255	38.582	1.00 65.91
ATOM	2779				806	32.435	20.046	40.089	
MOTA	2780				806	32.267			1.00 65.62
ATOM	2781				806		21.765	38.255	1.00 66.46
ATOM	2782					33.719	20.639	40.611	1.00 65.48
ATOM	2783	N			813	29.912	8.313	36.265	1.00 60.30
		CA			813	30.605	8.781	35.059	1.00 60.57
ATOM	2784	С			813	29.707	9.617	34.157	1.00 60.31
ATOM	2785	0			813	28.484	9.496	34.194	1.00 60.27
ATOM	2786	CB			813	31.167	7.599	34.266	1.00 60.46
MOTA	2787	CG	LEU	S	813	32.067	6.674	35.092	1.00 60.30
MOTA	2788	CD1	LEU	s	813	32.450	5.418	34.281	1.00 61.04
ATOM	2789				813	33.301	7.421	35.602	1.00 59.11
ATOM .	2790	N			814	30.344	10.465	33.355	
ATOM	2791	CA			814	29.648			1.00 60.31
ATOM	2792	C			814		11.353	32.440	1.00 60.05
ATOM	2793	Õ				30.557	11.803	31.295	1.00 59.62
ATOM	2794				814	31.765	11.584	31.322	1.00 58.97
ATOM	2795	CB			814	29.176	12.583	33.194	1.00 60.41
		CG				30.302	13.488	33.634	1.00 62.13
MOTA	2796	CD			814	29.826	14.603	34.559	1.00 64.43
ATOM	2797		GLN			29.260	14.327	35.616	1.00 65.48
ATOM	2798		GLN			30.058	15.859	34.167	1.00 65.06
ATOM	2799	N			815	29.960	12.456	30.302	1.00 59.55
ATOM	2800	CA.			815	30.675	12.927	29.136	1.00 59.21
MOTA	2801	С	GLY	S	815	31.493	11.823	28.493	1.00 59.26
MOTA	2802	Ó	GLY	S	815	31.049	10.678	28.399	1.00 58.48
MOTA	2803	N	GLU	S	816	32.693	12.183	28.049	1.00 59.73
ATOM	2804	CA	GLU	S	816	33.604	11.254	27.392	1.00 60.76
MOTA	2805	С			816	33.768	9.941	28.168	1.00 61.61
ATOM	2806	0	GLU			33.861	8.866	27.567	
ATOM	2807	ĊВ			816	34.978	11.913		1.00 61.64
ATOM	2808	ĊG			816	35.802	11.304	27.190 26.064	1.00 60.71
MOTA	2809	CD			816	37.208	11.872		1.00 61.12
MOTA	2810		GLU			38.066		25.979	1.00 61.35
ATOM	2811		GLU			37.467	11.370	26.730	1.00 61.67
ATOM	2812	N			817		12.801	25.168	1.00 60.68
ATOM	2813	CA			817	33.791	10.030	29.495	1.00 62.56
ATOM	2814					33.962	8.851	30.332	1.00 63.66
		C			817	32.748	7.929	30.260	1.00 63.92
ATOM	2815	0	GLU			32.887	6.709	30.187	1.00 63.68
ATOM	2816	CB			817	34.217	9.257	31.777	1.00 63.99
MOTA	2817	CG			817	35.518	10.012	31.974	1.00 65.72
MOTA	2818	CD	GLÜ			35.371	11.514	31.786	1.00 69.17
ATOM	2819		GLU			34.253	11.990	31.452	1.00 70.86
ATOM	2820	OE2				36.384	12.228	31.984	1.00 71.76
ATOM	2821	N	LEU			31.558	8.517	30.296	1.00 64.38
MOTA	2822	CA	LEU			30.344	7.733	30.191	1.00 64.38
MOTA	2823	С	LEU			30.367	6.935	28.890	1.00 65.31
MOTA	2824	0	LEU			30.166	5.723	28.901	1.00 65.31
ATOM	2825	СВ	LEU			29.092	8.624	30.232	
ATOM	2826	CG	LEU			27.770	7.844	30.232	1.00 64.90
		-		_	-	_,,,,		20.102	1.00 64.94

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ATOM 2	2827	CD1	LEU S	818	27.702	6.871	31.316	1.00 6	6.53	c	:
			LEU S		26.551		30.205	1.00 6		C	
	2829		LEU S		30.647	•	27.787	1.00		Ŋ	
	2830		LEU S		30.608		26.445	1.00		C	
	2831		LEU S		31.569	5.851	26.294	1.00		Ċ	3
	2832		LEU S		31.174	4.773	25.852	1.00)
	2833		LEU S		30.901	8.122	25.392	1.00			2
	2834		LEU S		30.860	7.737	23.916	1.00		Č	-
	2835		LEU S		29.537	7.149	23.501	1.00			C
	2836		LEU S		31.162	8.967	23.083	1.00			C
	2837		ARG S		32.820	6.053	26.684	1.00			N
	2838		ARG S		33.824	5.013	26.561	1.00			C
	2839		ARG S		33.492	3.801	27.432	1.00			C
			ARG S		33.573	2.643	26.969	1.00			0
	2841		ARG S		35.196	5.574	26.917	1.00			C
	2842		ARG S		35.628	6.605	25.907	1.00			C
	2843	CD	ARG S		37.048	7.061	26.030	1.00			C
	2844	NE	ARG S		37.309	8.138	25.079	1.00			N
	2845	CZ	ARG S		38.442	8.839	25.014	1.00			C
ATOM ATOM	2846		ARG S		39.451	8.581	25.851		75.90		N
	2847		ARG S		38.566	9.806	24.104		75.55		N
ATOM ATOM	2848	Nnz	ALA S		33.118	4.067	28.684				
MOTA	2849	CA	ALA S		32.712	2.999	29.580		66.99		C
ATOM	2850	C	ALA S		31.609	2.171	28.898		66.76		C
ATOM	2851	0	ALA S		31.660	0.945	28.889		66.63		Ō
ATOM	2852	CB	ALA S		32.234	3.562	30.901		66.88		C
	2853	N	LEU S		30.625	2.851	28.313		66.58		N
MOTA MOTA	2854	CA	LEU S		29.538	2.173	27.607		66.36		С
ATOM	2855	C	LEU S		30.027	1.439	26.359		66.21	•	C
	2856	o	LEU S		29.429	0.444	25.956		66.11		ō
MOTA	2857	СВ		5 822 5 822	28.451		. 27.223		66.06		Ċ
ATOM ATOM	2858	CG		822	27.710	3.789	28.406		65.45		C
ATOM	2859		LEUS		26.559	4.613	27.885		65.37		С
ATOM	2860		LEU		27.213	2.732	29.396		65.08		С
TER	2861	CDZ		S 822	27.215	2.,02	23.030				
HETATM		ZN		A1350	23.324	27.578	28.817	1.00	32.29	:	ZN
HETATM		C1		A1351	22.262	25.308	27.891		34.79		C.
HETATM		C2		A1351	21.209	25.940	28.487		32.90		С
HETATM		C4		A1351	18.882	25.730	29.253		32.24		C
HETATM		.C5		A1351	17.543	25.251	28.735		32.20		С
HETATM		01		A1351	22.091	24.207	27.399		33.47		0
HETATM				A1351			27.813	1.00	33.83		0
HETATM				A1351	21.299	27.077	29.004		31.02		0
HETATM				A1351	17.430	24.476	27.795	1.00	33.67		0
HETATM				A1351	20.067	25.271		1.00	29.83		N
HETATM				A1351	16.551	25.641		1.00	32.21	•	0
HETATM				A1352	0.290	25.194	43.827	1.00	90.02		S
HETATM				A1352	1.120	26:025			89.95		0
HETATN				A1352	1.151	24.261		1.00	88.91		0
HETATN				A1352	-0.627	24.447	44.672	1.00	90.38		0
HETAT				A1352	-0.468	26.028	42.891		89.30		0
HETAT				A1353	1.893	28.515	29.870	1.00	98.62		S
HETATI				A1353	3.138	29.102		1.00	97.69		0
HETATE				A1353	2.145	27.399	28.947		97.91		0
HETATI		-		A1353	1.205	28.059		1.00	99.26		0
HETATI				A1353	1.078	29.515	29.171		98.46		0
HETAT			нон		38.820	33.858	31.965		46.43		0
HETAT			HOH		33.795	30.509	39.255		71.93		0
HETATI			HOH		34.891	30.536			48.26		0
HETAT	м 2886	5 0	нон	H 4	35.615	13.844			48.67		0
HETAT	M 2887	7 0	нон	Z 1	11.592	21.463	13.878	3 1.00	49.06		0

HETATM	2888	0	HOH	Z	2	9.700	21.662	.12.247	1.00 70.56	0
HETATM	2889	0	HOH	Z	3	1.136	21.407	7.962	1.00 66.59	0
HETATM	2890	0	нон	\mathbf{z}	4	2.407	19.370	5.351	1.00 60.28	Ō
HETATM	2891	0	HOH	Z	5	1.014	29.292	13.196	1.00 61.25	o .
HETATM	2892	0	HOH	Z	6	2.256	32.365	14.166	1.00 73.91	Ō
HETATM	2893	0	HOH	Z	7	11.526	44.954	15.330	1.00 68.94	Ö
HETATM	2894	0	НОН	Z	8	-1.438	30.257	22.663	1.00 85.46	Ö
'HETATM	2895	0	нон		9	7.738	30.579	27.736	1.00 46.83	Ö
HETATM	2896	0	нон		10	3.543	32.597	32.323	1.00 73.21	ō
HETATM	2897	0	нон		11	6.618	43.722	26.114	1.00 79.20	Ö
HETATM	2898	0	нон		12	4.723	37.184	27.600	1.00 69.48	ŏ
HETATM	2899	0	нон		13	10.942	35.610	30.382	1.00 48.93	Ö
HETATM	2900	0	НОН		14	13.888	48.615	19.570	1.00 55.60	Ö
HETATM		0	нон		15	12.153	41.664	15.818	1.00 61.09	ő
HETATM	2902	0	нон		16	15.898	30.602	12.921	1.00 48.84	Ö
HETATM	2903	0	нон		17	13.629	22.042	7.314	1.00 56.45	Ö
HETATM		0	нон		18	14.608	26.242	13.702	1.00 55.84	Ö
HETATM		Ō	НОН		19	21.110	23.978	3.732	1.00 33.84	0
HETATM		ō	нон		20	22.517	24.246	0.061	1.00 58.70	0
HETATM		ŏ	нон		21	27.322	30.745	5.813	1.00 38.70	
HETATM		ŏ	нон		22	26.669	21.831	43.291	1.00 71.25	, 0
HETATM		Ö	нон		23	36.928	29.423	21.116		0
HETATM		Õ	нон		24	28.560	37.933	15.396	1.00 60.53	0
HETATM		Ö	нон		25	29.71.7	37.933	10.091	1.00 65.84 1.00 70.57	0
HETATM		ŏ	нон		26	19.889				0
HETATM		Ö	нон		27	18.190	17.921	13.411	1.00 40.68	0
HETATM		Ö	нон	_	28	19.229	15.068	13.047	1.00 45.64	0
HETATM		0	НОН		29		14.479	16.581	1.00 44.23	0
HETATM		0	НОН			5.509	12.781	28.209	1.00 48.58	0
HETATM		0			30	19.118	6.397	36.829	1.00 62.79	0
HETATM		0	НОН		31	33.446	44.026	25.377	1.00 68.72	0
HETATM		.0	НОН		32	8.427	26.875	44.426	1.00 65.85	0
HETATM		_	НОН		33	9.122	31.413	42.815	1.00 79.14	0
HETATM		0	HOH		34	15.645	37.855	35.686	1.00 55.81	0
HETATM		0	НОН		35	16.264	30.912	40.283	1.00 52.67	0
HETATM		0	нон		36	28.580	24.804	42.231	1.00 71.47	0
HETATM		0	НОН		37	25.125	24.702	42.513	1.00 61.76	0
		0	НОН		38	31.710	33.903	46.336	1.00 58.86	0
HETATM		0	НОН		39	24.430	38.695	49.842	1.00 64.87	0
HETATM		0	нон		40	21.999	17.349	48.274	1.00 78.90	0
HETATM		0	НОН		41	22.174	10.277	34.700	1.00 61.90	0
HETATM		0	НОН		42	17.917	-1.798	33.038	1.00 69.51	0
HETATM		0	нон		43	36.654	10.887	7.525	1.00 72.57	0
HETATM		0	нон		44	13.628	20.833	28.536	1.00 46.20	0
HETATM		0	нон		45	3.910	21.434	31.018	1.00 60.17	0
HETATM		0	нон		46	30.778	38.131	33.414	1.00 33.59	0
HETATM		0	НОН		47	25.976	26.458	26.213	1.00 38.20	0
HETATM		0	НОН		48	· 35.876	25.491	27.760	1.00 47.36	0
HETATM		0	НОН		49	36.704	26.679	21.111	1.00 49.53	0
HETATM		0	НОН		50	17.375	16.970	18.001	1.00 37.06	0
HETATM		0	нон		51	5.442	16.762	21.954	1.00 48.45	0
HETATM		0	НОН		52	6.786	12.615	22.641	1.00 71.97	0
HETATM		0	HOH		53	7.201	17.017	20.359	1.00 48.19	0
HETATM		0	нон		54	6.512	22.748	23.330	1.00 52.43	. 0
HETATM		0	НОН		·55	29.528	38.794	26.547	1.00 33.74	0
HETATM		0	НОН		56	30.683	39.271	19.412	1.00 42.04	0
HETATM		0	нон		57	26.571	42.213	18.009	1.00 59.45	0
HETATM		0	HOH		58	29.038	40.259	16.007	1.00 65.33	0
HETATM		0	HOH		59	27.631	44.557	31.407	1.00 36.71	0
HETATM		0	HOH		60	27.654	48.738	30.067	1.00 46.82	0
HETATM		0	HOH	Z	61	30.426	45.052	25.424	1.00 49.55	Ō
HETATM	2948	0	НОН	Z	62	25.946	50.745	30.903	1.00 51.76	Ō
						•				_

HETATM :	2949	0	HOH Z	63	2	26.759	31.212		1.00				
HETATM :	2950	0	HOH Z	64	2	29.563	36.988	35.538	1.00	36.	. 58		
HETATM :	2951	0	HOH Z	65	3	30.608	30.268	36.508	1.00	39.	. 97		
HETATM		0	HOH Z	66		19.823	31.620	33.966	1.00	44.	. 64		
HETATM	2953		нон Z	67		19.517	36.182	33.531	1.00	39	. 38		
HETATM			нон 2	68		18.255	38.678	36.813	1.00				
HETATM			нон Z	69		21.026	42.838	40.240	1.00				
HETATM			HOH Z	70		17.610	37.832	32.310	1.00				
HETATM			HOH Z	71		15.109	37.973	32.827	1.00				
HETATM			HOH Z	72		16.418	47,375	39.219	1.00				
HETATM		ŏ	HOH Z	73		15.605	44.895	35.040	1.00				
HETATM		0	HOH Z					27.660	1.00		•		
			HOH Z			15.476		22.363	1.00				
HETATM		0						22.198	1.00				
HETATM		0	HOH Z			16.645	46.682						
HETATM		0	HOH Z				40.795	15.622	1.00				
HETATM			HOH Z			10.674	19.290	14:058	1.00				
HETATM		0	HOH Z			27.773	27.556	24.476	1.00				
HETATM		0 .	HOH Z			30.214		27.011	1.00				
HETATM		0	HOH Z				34.179	19.369	1.00				
HETATM		0	HOH Z				30.221		1.00				
HETATM		0	HOH Z			16.261							
HETATM		0	HOH Z				23.973		1.00				
HETATM		0	нон z			4.061			1.00				
HETATM		0	HOH Z			42.841			1.00				
HETATM		0	HOH Z				44.259		1.00				
HETATM		0	HOH Z			33.750							
HETATM		0	HOH Z			33.208							
HETATM		0	HOH Z				40.251						
HETATM	2977	0	HOH Z				43.762						
HETATM	2978	0	HOH Z				57.294						
HETATM	2979	0	HOH Z	3 93			.53.378						
HETATM	2980	0	HOH Z	3 94			55.476						
HETATM	2981	0	HOH Z	2 95		38.489	59.800	33.014	1.00) 55	5.47		
CONECT	1478	2862							•	•			
CONECT	1498	2862											
CONECT	2167	2862					•					-	
CONECT	2862	2869	2868	1478	2167	1498							
CONECT	2863	2864	2867	2868									
CONECT	2864	2863	2869	2871		٠.							
CONECT	2865	2866	2871										
CONECT	2866	2865	2870	2872									
CONECT	2867	2863	3										
CONECT	2868	2863	3 2862										
CONECT	2869	2864	2862										
CONECT	2870	2866	5										
CONECT	2871	2864	2865										
CONECT	2872	2866	5										
CONECT	2873	2874	2875	2876	2877								
CONECT													
CONECT													
CONECT													
CONECI													
CONECI				2881	2882								
CONECT					_002	-							
CONECI													
CONECT													
CONECT													
MASTER		446		. 4	15	20	0 8	6 297	19	2	24	31	
END			•	-2				Ç 23'	-	-			

Structure 4

Below are the coordinates for structure 4 (the 2.85 Å structure of FIH:Fe(II):20G):

```
HEADER
          TRANSCRIPTION ACTIVATOR/INHIBITOR
                                                    12-AUG-02
                                                                 1H2N
TITLE
          FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX WITH HIF-1 ALPHA
TITLE
         2 FRAGMENT PEPTIDE
COMPND
         MOL ID: 1;
COMPND
         2 MOLECULE: FACTOR INHIBITING HIF1;
COMPND
         3 SYNONYM: FIH1;
COMPND
         4 CHAIN: A;
COMPND
         5 ENGINEERED: YES
SOURCE
         MOL ID: 1;
SOURCE
         2 ORGANISM SCIENTIFIC: HOMO SAPIENS;
SOURCE
         3 ORGANISM COMMON: HUMAN;
SOURCE
         4 EXPRESSION SYSTEM: ESCHERICHIA COLI;
SOURCE
         5 EXPRESSION_SYSTEM STRAIN: BL21(DE3);
SOURCE
         6 EXPRESSION SYSTEM PLASMID: PET28A(+)
KEYWDS
          FIH, HIF, DSBH, OXYGENASE, TRANSCRIPTION, HYPOXIA,
         2 2-OXOGLUTARATE, ASPARAGINYL HYDROXYLASE, HYDROXYLASE
KEYWDS
EXPDTA
          X-RAY DIFFRACTION
          J.M.ELKINS, K.S.HEWITSON, L.A.MCNEILL, I.SCHLEMMINGER,
AUTHOR
AUTHOR
         2 J.F.SEIBEL, C.J.SCHOFIELD
REVDAT
             04-SEP-02 1H2N
JRNL
            AUTH
                    J.M.ELKINS, K.S.HEWITSON, L.A.MCNEILL,
JRNL
            AUTH 2 I.SCHLEMMINGER, J.F. SEIBEL, C.J. SCHOFIELD
JRNL
                    FIH: HIF-FRAGMENT COMPLEXES
JRNL
            REF
                    TO BE PUBLISHED
JRNL
            REFN
REMARK
         2 RESOLUTION. 2.84 ANGSTROMS.
REMARK
REMARK
         3
REMARK
         3 REFINEMENT.
REMARK
         3
             PROGRAM
                          : REFMAC 5.0
REMARK
         3
             AUTHORS
                          : MURSHUDOV, VAGIN, DODSON
REMARK
         3
REMARK
         3
              REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK
         3
REMARK
         3
            DATA USED IN REFINEMENT.
REMARK
         3
             RESOLUTION RANGE HIGH (ANGSTROMS) :
                                                      2.84
REMARK
         3
             RESOLUTION RANGE LOW
                                     (ANGSTROMS) :
                                                     30.00
REMARK
         3
              DATA CUTOFF
                                      (SIGMA(F)) : NONE
REMARK
         3
              COMPLETENESS FOR RANGE
                                              (용) :
                                                    99.51
REMARK
         3
              NUMBER OF REFLECTIONS
                                                      12577
REMARK
         3
REMARK
         3
             FIT TO DATA USED IN REFINEMENT.
              CROSS-VALIDATION METHOD
REMARK
         3
                                                 : THROUGHOUT
REMARK
              FREE R VALUE TEST SET SELECTION
                                                : RANDOM
REMARK
                           (WORKING + TEST SET) : 0.23287
              R VALUE
REMARK
         3
              R VALUE
                                  (WORKING SET)
                                                   0.23094
REMARK
         3
              FREE R VALUE
                                                    0.25695
REMARK
         3
              FREE R VALUE TEST SET SIZE
                                                    7.7
                                             (8):
REMARK
         3
              FREE R VALUE TEST SET COUNT
                                                    1046
REMARK
         3
REMARK
         3
             FIT IN THE HIGHEST RESOLUTION BIN.
REMARK
         3
              TOTAL NUMBER OF BINS USED
                                                           20
REMARK
         3
              BIN RESOLUTION RANGE HIGH
                                                         2.840
REMARK
         3
              BIN RESOLUTION RANGE LOW
                                                         2.913
REMARK
              REFLECTION IN BIN
                                     (WORKING SET) :
                                                           828
```

```
(WORKING SET) :
            BIN R VALUE
REMARK
        3
            BIN FREE R VALUE SET COUNT
REMARK
            BIN FREE R VALUE
REMARK
REMARK
        3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK
                            : 2689
REMARK
            PROTEIN ATOMS
                                    : 0
            NUCLEIC ACID ATOMS
REMARK
                                    : 26
            HETEROGEN ATOMS
REMARK
            SOLVENT ATOMS
                                    : 3
REMARK
        3
REMARK
REMARK
        3 B VALUES.
                                      (A**2) : NULL
           FROM WILSON PLOT
REMARK
        3
           MEAN B VALUE (OVERALL, A**2): 35.345
REMARK
        3 · OVERALL ANISOTROPIC B VALUE.
REMARK
            B11 (A**2) : -1.02
REMARK
        3
             B22 (A**2):
                             -1.02
REMARK
        3
            B33 (A**2) :
                              2.03
         3
REMARK
             B12 (A**2) :
                              0.00
REMARK
         3
             B13 (A**2) :
REMARK
         3
                              0.00
             B23 (A**2) :
                             0.00
REMARK
         3
REMARK
         3
           ESTIMATED OVERALL COORDINATE ERROR.
REMARK
         3
                                                                   0.852
       . 3
            ESU BASED ON R VALUE
                                                            (A):
REMARK
             ESU BASED ON FREE R VALUE
                                                            (A):
REMARK
                                                                   0.398
             ESU BASED ON MAXIMUM LIKELIHOOD
                                                             (A):
REMARK
             ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2):
REMARK
         3
        ٠3
REMARK
         3 CORRELATION COEFFICIENTS.
REMARK
            CORRELATION COEFFICIENT FO-FC
                                                  0.913
REMARK
             CORRELATION COEFFICIENT FO-FC FREE: 0.901
 REMARK
 REMARK
         3 RMS DEVIATIONS FROM IDEAL VALUES
                                                   COUNT
                                                           RMS
 REMARK
                                               (A): 2791; 0.015; 0.021
            BOND LENGTHS REFINED ATOMS
 REMARK
         3
                                               (A): 2388; 0.001; 0.020
 REMARK
         3
             BOND LENGTHS OTHERS
            BOND ANGLES REFINED ATOMS (DEGREES): 3799; 1.628; 1.945
 REMARK
         3
                                       (DEGREES): 5576; 0.823; 3.000
            BOND ANGLES OTHERS
 REMARK
           CHIRAL-CENTER RESTRAINTS

GENERAL PLANES REFINE

CHIRAL-CENTER RESTRAINTS

GENERAL PLANES REFINE

GENERAL PLANES REFINE

GENERAL PLANES REFINE

CHIRAL-CENTER RESTRAINTS
         3
                                                    330 ; 4.268 ; 3.000
 REMARK
         3
                                                     479 ;18.082 ;15.000
 REMARK
         3
                                                     384 ; 0.095 ; 0.200
 REMARK 3
                                                    3137 ; 0.005 ; 0.020
 REMARK · 3
                                               (A):
                                                     575 ; 0.002 ; 0.020
             GENERAL PLANES OTHERS
 REMARK 3
                                                     717 ; 0.255 ; 0.300
         3 NON-BONDED CONTACTS REFINED ATOMS (A):
 REMARK
         3 NON-BONDED CONTACTS OTHERS (A): 2425; 0.224; 0.300
 REMARK
          3 H-BOND (X...Y) OTHERS (A):
3 POTENTIAL VIEW
                                                      165 ; 0.139 ; 0.500
 REMARK 3 H-BOND (X...Y) REFINED ATOMS
                                                     1 ; 0.102 ; 0.500
 REMARK
              POTENTIAL METAL-ION REFINED ATOMS (A):
                                                       3 ; 0.112 ; 0.500
 REMARK
          3
                                                     14 ; 0.256 ; 0.300
              SYMMETRY VDW REFINED ATOMS (A):
 REMARK
          3
                                                (A): 62; 0.273; 0.300
              SYMMETRY VDW OTHERS
 REMARK
          3
              SYMMETRY H-BOND REFINED ATOMS
                                               (A): 4 ; 0.214 ; 0.500
 REMARK
          3
                                                       1 ; 0.061 ; 0.500
 REMARK
          3
              SYMMETRY H-BOND OTHERS
                                               (A):
 REMARK
                                                    COUNT RMS
             ISOTROPIC THERMAL FACTOR RESTRAINTS.
                                                                   WEIGHT
 REMARK
              MAIN-CHAIN BOND REFINED ATOMS (A**2): 1659; 0.312; 1.500
 REMARK
              MAIN-CHAIN ANGLE REFINED ATOMS (A**2): 2675; 0.598; 2.000
 REMARK
              SIDE-CHAIN BOND REFINED ATOMS (A**2): 1132; 1.058; 3.000
 REMARK
              SIDE-CHAIN ANGLE REFINED ATOMS (A**2): 1124 ; 1.795 ; 4.500
  REMARK
  REMARK
  REMARK
          3 NCS RESTRAINTS STATISTICS
             NUMBER OF NCS GROUPS : NULL
  REMARK
         3
          3
  REMARK
         3 TLS DETAILS
  REMARK
```

```
REMARK
            NUMBER OF TLS GROUPS : 1
        3
REMARK
        3
REMARK
        3 TLS GROUP:
                            1
        3 NUMBER OF COMPONENTS GROUP: 1
REMARK
           COMPONENTS C SSSEQI TO C SSSEQI
RESIDUE RANGE: A 15 A 452
REMARK
        3
        3 RESIDUE RANGE : A 15
REMARK
        3 ORIGIN FOR THE GROUP (A): 21.4490 27.4200 27.7870
REMARK
        3 T TENSOR
REMARK
            T11:
T33:
                      0.2230 T22:
REMARK
                                    0.0562
                    0.0967 T12:
REMARK
                                   0.0111
REMARK
        3
              T13: -0.0923 T23:
                                  0.0525
        3 L TENSOR
REMARK
            L11:
REMARK 3
                      1.6842 L22:
                                    4.4489
REMARK
        3
             L33:
                      2.0658 L12:
                                    1.5597
           · L13:
REMARK
        3
                      1.1572 L23: 2.3523
REMARK
           S TENSOR
        3
                      0.1098 S12: -0.2106 S13: -0.0766
REMARK
         3
             S11:
                      0.3449 S22: -0.0455 S23:
REMARK
         3
               S21:
                                                0.2455
REMARK
         3
               S31:
                      0.3515 S32: -0.1199 S33: -0.0643
REMARK
         3
         3 BULK SOLVENT MODELLING.
REMARK
REMARK
         3. METHOD USED .: BABINET MODEL WITH MASK
       3
3
3
3
REMARK
         3
            PARAMETERS FOR MASK CALCULATION
REMARK
                              : 1.40
            VDW PROBE RADIUS
REMARK
            ION PROBE RADIUS
                                   0.80
REMARK
            SHRINKAGE RADIUS
                                   0.80
REMARK
       3 OTHER REFINEMENT REMARKS: SEE REMARK 400
REMARK
REMARK
. REMARK
       4 1H2N COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY EBI ON 12-AUG-2002.
REMARK 100 THE EBI ID CODE IS EBI-11174.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE
           EXPERIMENT TYPE : X-RAY DIFFRACTION DATE OF DATA COLLECTION : 15-MAY-2002
REMARK 200
REMARK 200 TEMPERATURE
                                (KELVIN) : 100
REMARK 200 PH
                                        : 7.5
REMARK 200
           NUMBER OF CRYSTALS USED
REMARK 200
                              (Y/N) : Y
REMARK 200 SYNCHROTRON
REMARK 200
                                          : SRS BEAMLINE PX9.5
           RADIATION SOURCE
REMARK 200
           BEAMLINE
                                          : PX9.5
REMARK 200
           X-RAY GENERATOR MODEL
                                         : NULL
            MONOCHROMATIC OR LAUE (M/L) : M
REMARK 200
REMARK 200
            WAVELENGTH OR RANGE
                                     (A) : 0.92
            MONOCHROMATOR
REMARK 200
                                          : NULL
REMARK 200
            OPTICS
                                          : NULL
REMARK 200
REMARK 200
            DETECTOR TYPE
                                          : MARCCD
                                   : MARRESEARCH
REMARK 200
            DETECTOR MANUFACTURER
REMARK 200
            INTENSITY-INTEGRATION SOFTWARE : MOSFLM
REMARK 200
            DATA SCALING SOFTWARE
                                         : SCALA
REMARK 200
            NUMBER OF UNIQUE REFLECTIONS : 13703
REMARK 200
            RESOLUTION RANGE HIGH (A): 2.84 RESOLUTION RANGE LOW (A): 34.1
REMARK 200
REMARK 200
REMARK 200
            REJECTION CRITERIA (SIGMA(I)) : NONE
REMARK 200
REMARK 200 OVERALL.
```

```
(%): 99.2
REMARK 200 COMPLETENESS FOR RANGE
                                                  : 6.7
REMARK 200 DATA REDUNDANCY
                                               (I): 0.067
REMARK 200 R MERGE
REMARK 200 R SYM
                                               (I) : NULL
REMARK 200 <1/SIGMA(I)> FOR THE DATA SET : 9.4
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.84
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A): 2.99
REMARK 200 COMPLETENESS FOR SHELL (%): 94.9
                                               : 5.2
             DATA REDUNDANCY IN SHELL
REMARK 200
                                              (I) : 0.309
REMARK 200 R MERGE FOR SHELL
                                              (I) : NULL
REMARK 200 R SYM FOR SHELL
REMARK 200
              <!/SIGMA(I)> FOR SHELL
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR REPLACEMENT
REMARK 200 SOFTWARE USED: NULL
REMARK 200 STARTING MODEL: NULL
REMARK 200
 REMARK 200 REMARK: SEE REMARK 400
 REMARK 280
 REMARK 280 CRYSTAL
 REMARK 280 SOLVENT CONTENT, VS (%): 63
 REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 3.4
 REMARK 280
 REMARK 280 CRYSTALLIZATION CONDITIONS: 1.2M AMMONIUM SULPHATE,
 REMARK 280 4% PEG400, 0.1M HEPES PH7.5 ARGON ATMOSPHERE,
 REMARK 280 11MG/ML PROTEIN WITH 1MM FE(II), 2.5MM AKG AND 2.5MM
 REMARK 280 PEPTIDE (SEE REMARK 400)
 REMARK 290
 REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
 REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 41 21 2
 REMARK 290
                   SYMOP SYMMETRY
 REMARK 290
                 NNNMMM OPERATOR
 REMARK 290
                  1555 X,Y,Z
 REMARK 290
 REMARK 290
                   2555 - X, -Y, 1/2 + Z
                 3555 -x,-Y,1/2+Z

3555 1/2-Y,1/2+X,1/4+Z

4555 1/2+Y,1/2-X,3/4+Z

5555 1/2-X,1/2+Y,1/4-Z

6555 1/2+X,1/2-Y,3/4-Z

7555 Y,X,-Z
 REMARK 290
 REMARK 290
 REMARK 290
 REMARK 290
  REMARK 290
                    8555
                           -Y, -X, 1/2-Z
  REMARK 290
  REMARK 290
  REMARK 290 WHERE NNN -> OPERATOR NUMBER
                          MMM -> TRANSLATION VECTOR
  REMARK 290
  REMARK 290
  REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
  REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
  REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
  REMARK 290 RELATED MOLECULES.
                 SMTRY1 1 1.000000 0.000000 0.000000
                                                                           0.00000
  REMARK 290
                            1 0.000000 1.000000 0.000000
                                                                           0.00000
                 SMTRY2
  REMARK 290
                 SMTRY3
                            1 0.000000 0.000000 1.000000
  REMARK 290
                            2 -1.000000 0.000000 0.000000
                 SMTRY1
  REMARK 290

      SMTRY1
      2 -1.000000
      0.000000
      0.000000

      SMTRY2
      2 0.000000
      -1.000000
      0.000000

      SMTRY3
      2 0.000000
      0.000000
      1.000000

      SMTRY1
      3 0.000000
      -1.000000
      0.000000

      SMTRY2
      3 1.000000
      0.000000
      0.000000

      SMTRY3
      3 0.000000
      0.000000
      1.000000

  REMARK 290
  REMARK 290
  REMARK 290
                                                                         43.17100
  REMARK 290
  REMARK 290
```

```
REMARK 290
            SMTRY1 4 0.000000 1.000000 0.000000
                                                           43.17100
            SMTRY2
REMARK 290
                     4 -1.000000 0.000000 0.000000
                                                           43.17100
REMARK 290
            SMTRY3
                     4 0.000000 0.000000
                                           1.000000
                                                          110.04900
                                  0.000000 0.000000
REMARK 290
            SMTRY1
                     5 -1.000000
                                                           43.17100
REMARK 290
            SMTRY2
                     5 0.000000
                                  1.000000
                                           0.000000
                                                           43.17100
REMARK 290
                     5 0.000000 0.000000 -1.000000
            SMTRY3
                                                           36.68300
REMARK 290
                                            0.000000
            SMTRY1
                     6
                        1.000000 0.000000
                                                           43.17100
                        0.000000 -1.000000
REMARK 290
           · SMTRY2
                                            0.000000
                     6
                                                           43.17100
REMARK 290
            SMTRY3
                        0.000000 0.000000 -1.000000
                     6
                                                           110.04900
                         0.000000 1.000000
REMARK 290
                     7
                                            0.000000
            SMTRY1
                                                            0.00000
REMARK 290
            SMTRY2
                     7
                                            0.000000
                         1.000000 0.000000
                                                             0.00000
REMARK 290
            SMTRY3
                     7
                         0.000000 \quad 0.000000 \quad -1.000000
                                                             0.00000
REMARK 290
             SMTRY1
                     8
                        0.000000 -1.000000 0.000000
                                                            0.00000
                     8 -1.000000 0.000000 0.000000
REMARK 290
             SMTRY2
                                                            0.00000
REMARK 290
                     8 0.000000 0.000000 -1.000000
             SMTRY3
                                                            73.36600
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
REMARK 300 WHICH CONSISTS OF 2 CHAIN(S). SEE REMARK 350 FOR
REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
REMARK 300
REMARK 300 QUATERNARY STRUCTURE FOR THIS ENTRY: DIMERIC
REMARK 300
REMARK 300 THE PROTEIN IS A HOMODIMER FORMED BY CHAIN A.
REMARK 300
REMARK 300 FOR THE HOMO-ASSEMBLY DESCRIBED BY REMARK 350
REMARK 300 THE DIFFERENCE IN ACCESSIBLE SURFACE AREA PER
REMARK 300 CHAIN BETWEEN THE ISOLATED CHAIN AND THAT FOR
REMARK 300 THE CHAIN IN THE COMPLEX IS 1600.4 ANGSTROM**2
REMARK 350
REMARK 350 GENERATING THE BIOMOLECULE
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE: 1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A
REMARK 350
             BIOMT1 1 1.000000 0.000000 0.000000
                                                             0.00000
                     1 0.000000 1.000000 0.000000
REMARK 350
             BIOMT2
                                                             0.00000
             BIOMT3 1 0.000000 0.000000
REMARK 350
                                             1.000000
                                                             0.00000
REMARK 350
             BIOMT1
                      2 0.000000 -1.000000
                                             0.000000
                                                            86.34200
             BIOMT2
REMARK 350
                      2 -1.000000 0.000000 0.000000
                                                            86.34200
REMARK 350
                      2 0.000000 0.000000 -1.000000
             BIOMT3
                                                            73.36600
REMARK 400
REMARK 400 COMPOUND
REMARK 400
 REMARK 400
            THE PROTEIN (CHAIN A) WAS CRYSTALLIZED IN THE PRESENCE
 REMARK 400
            OF A PEPTIDE FRAGEMENT FROM ENDOTHELIAL PAS DOMAIN PROTEIN 1
 REMARK 400
            SWISS-PROT ID Q99814 (RESIDUES 846-858) BUT NONE OF THE
 REMARK 400
            RESIDUES CORRESPONDING TO THE PEPTIDE WERE VISIBLE IN THE
 REMARK 400
            ELECTRON DENSITY MAPS. IT IS POSSIBLE THAT THE PEPTIDE DID
 REMARK 400
            NOT BIND TO THE PROTEIN AND HENCE HAS NOT BEEN INCLUDED IN THE
 REMARK 400
            COMPND, SOURCE AND SEQRES RECORDS.
 REMARK 400
 REMARK 400
            THE SEQUENCE OF THE FRAGMENT IS GIVEN BELOW.
 REMARK 400
 REMARK 400
            VAL ASN VAL PRO VAL LEU GLY SER SER THR LEU LEU GLN
```

```
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
             M RES C SSSEQI
REMARK 465
REMARK 465
               MET A
                          1
                          2
REMARK 465
               ALA A
                          3
REMARK 465
                ALA A
REMARK 465
                THR A
                ALA A
                          5
REMARK 465
                ALA A
                          6
REMARK 465
                GLU A
                          7
REMARK 465
REMARK 465
                ALA A
                          8
                          9
REMARK 465
                VAL A
                         .10
REMARK 465
                ALA A
REMARK 465
                SER A
                         11
REMARK 465
                GLY A
                         12
                SER A
                         13
REMARK 465
REMARK 465
                GLY A
                         14
REMARK 465
                LYS A
                         304
REMARK 465
                ARG A
                         305
                ILE A
                         306
REMARK 465
 REMARK 470
 REMARK 470 MISSING ATOM
 REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;
 REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;
 REMARK 470 I=INSERTION CODE):
              M RES CSSEQI ATOMS
 REMARK 470
                                   CD
                                         OE1
                                              OE<sub>2</sub>
               GLU A 15
                              CG
 REMARK 470
                GLU A 29
                              CG
                                   CD
                                         OE1
 REMARK 470
                                   OD1
                                        ND2
                ASN A 87
                              CG
 REMARK 470
                                   CE
                                         NZ
                              CD
 REMARK 470
                LYS A 106
                              CG
                                   CD .
                                         CE .
                                              NZ
               LYS A 115
 REMARK 470
                                         NE . CZ
                                                    NH1
                                                         NH2
               ARG A 117
                              CG
                                   CD
 REMARK 470
                                              NE2
                              CG
                                   CD
                                         OE1
 REMARK 470
               GLN A 133
                                         OE1
                                              NE2
 REMARK 470
               GLN A 136
                              CG
                                    CD
                              CG
                                    CD
                                         OE1 NE2
 REMARK 470
                 GLN A 137 ·
                                              CZ
                                                    NH1
                                                         NH2
                                         NE
 REMARK 470
                 ARG A 156
                              CG
                                    CD
                              CD
                                    CE
                                         NZ
 REMARK 470
                 LYS A 157
                                    CD
                                         CE
                                              NZ
                 LYS A 311
                               CG
 REMARK 470
 REMARK 500
 REMARK 500 GEOMETRY AND STEREOCHEMISTRY
 REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
 REMARK 500
 REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
 REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
  REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
  REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
  REMARK 500
  REMARK 500 STANDARD TABLE:
  REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 3(1X, A4, 2X), 12X, F5.1)
  REMARK 500
  REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
  REMARK 500
                                           EMTA
                                   ATM2
  REMARK 500
              M RES CSSEQI ATM1
                                               ANGL. DEV. = -10.1 DEGREES
                                 - CA - C
  REMARK 500
                 TYR A 261.
                            N
  REMARK 500
  REMARK 500 REMARK: NULL
  REMARK 500
```

```
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD AND BY MORE THAN 0.150 ANGSTROMS (M=MODEL
REMARK 500 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
REMARK 500 NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X, I3, 1X, A3, 1X, A1, I4, A1, 1X, 2(A4, A1, 3X), 12X, F5.3)
REMARK 500
REMARK 500 EXPECTED VALUESS: ENGH AND HUBER, 1991
REMARK 500
REMARK 500 M RES CSSEQI ATM1 RES CSSEQI ATM2 DEVIATION
                              MET A 343 CE
REMARK 500
             MET A 343 SD
                                                 -0.151
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
REMARK 500
REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
REMARK 500
 REMARK 500
           ATM1 RES C SSEQI
                                 ATM2 RES C SSEQI
                                                             DISTANCE
 REMARK 500
                          39
REMARK 500
             OG1 THR A
                                  OE1 GLU A 262
                                                                 2.16
REMARK 525
 REMARK 525 SOLVENT
 REMARK 525
 REMARK 525 THE SOLVENT MOLECULES ARE GIVEN CHAIN IDENTIFIERS TO
 REMARK 525 INDICATE THE PROTEIN CHAIN TO WHICH THEY ARE MOST CLOSELY
 REMARK 525 ASSOCIATED WITH:
 REMARK 525
            PROTEIN CHAIN SOLVENT CHAIN
 REMARK 525
 REMARK 600
 REMARK 600 HETEROGEN
 REMARK 600
 REMARK 600 FOR METAL ATOM FE FE2 A1350 THE COORDINATION ANGLES ARE:
 REMARK 600 1 HIS 199A NE2
 REMARK 600 2 ASP
                                   106.1
                   201A OD2
 REMARK 600 3 HIS
                   279A NE2
                                    77.8 85.5
                                   168.0 81.1 93.4
 REMARK 600 4 AKG 1351A 01
 REMARK 600 5 AKG 1351A 05
                                   88.7 163.3 90.2 83.1
 REMARK 600
                                       1
                                             2
                                                   3
 REMARK 700
 REMARK 700 SHEET
 REMARK 700 THE SHEET STRUCTURE OF THIS MOLECULE IS BIFURCATED. IN
 REMARK 700 ORDER TO REPRESENT THIS FEATURE IN THE SHEET RECORDS BELOW,
 REMARK 700 TWO SHEETS ARE DEFINED.
 REMARK 800
 REMARK 800 SITE
 REMARK 800 SITE IDENTIFIER: FEA
 REMARK 800 SITE DESCRIPTION: FE BINDING SITE FOR CHAIN A
 REMARK 800
 REMARK 800 SITE IDENTIFIER: AKG
 REMARK 800 SITE DESCRIPTION: AKG BINDING SITE FOR CHAIN A
 REMARK 800
 REMARK 800 SITE IDENTIFIER: SA1
 REMARK 800 SITE DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
 REMARK 800
```

```
REMARK 800 SITE IDENTIFIER: SA2
REMARK 800 SITE DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE IDENTIFIER: SA3
REMARK 800 SITE DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 1H2K
                              RELATED DB: PDB
REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1H2L
                              RELATED DB: PDB
REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1H2M RELATED DB: PDB
REMARK 900 FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900 WITH HIF-1 ALPHA FRAGMENT PEPTIDE
                     349 SWS
                                 Q969Q7
                                          Q969Q7
                                                                  349
       1H2N A
                 1
DBREF
              349 MET ALA ALA THR ALA ALA GLU ALA VAL ALA SER GLY SER
SEQRES
         1 A
                   GLY GLU PRO ARG GLU GLU ALA GLY ALA LEU GLY PRO ALA
SEORES
         2 A
              349
                   TRP ASP GLU SER GLN LEU ARG SER TYR SER PHE PRO THR
SEORES
         3 A
              349
                   ARG PRO ILE PRO ARG LEU SER GLN SER ASP PRO ARG ALA
SEQRES
         4 A
              349
                   GLU GLU LEU ILE GLU ASN GLU GLU PRO VAL VAL LEU THR
SEQRES
         5
           Α
              349
                   ASP THR ASN LEU VAL TYR PRO ALA LEU LYS TRP ASP LEU
SEQRES
         6 A
              349
                    GLU TYR LEU GLN GLU ASN ILE GLY ASN GLY ASP PHE SER
SEORES
         7 A
               349
                    VAL TYR SER ALA SER THR HIS LYS PHE LEU TYR TYR ASP
 SEORES
         8 A
               349
                    GLU LYS LYS MET ALA ASN PHE GLN ASN PHE LYS PRO ARG
 SEQRES
         9 A
               349
                    SER ASN ARG GLU GLU MET LYS PHE HIS GLU PHE VAL GLU
        10 A
               349
 SEQRES
                    LYS LEU GLN ASP ILE GLN GLN ARG GLY GLY GLU GLU ARG
               349
 SEQRES
        11 A
                    LEU TYR LEU GLN GLN THR LEU ASN ASP THR VAL GLY ARG
 SEQRES
        12 A
               349
                    LYS ILE VAL MET ASP PHE LEU GLY PHE ASN TRP ASN TRP
 SEQRES
        13 A
               349
                    ILE ASN LYS GLN GLN GLY LYS ARG GLY TRP GLY GLN LEU
 SEQRES
        14 A
               349
                    THR SER ASN LEU LEU LEU ILE GLY MET GLU GLY ASN VAL
 SEQRES
         15 A
               349
                    THR PRO ALA HIS TYR ASP GLU GLN GLN ASN PHE PHE ALA
         16 A
               349
 SEQRES
                    GLN ILE LYS GLY TYR LYS ARG CYS ILE LEU PHE PRO PRO
               349
         17 A
 SEORES
                    ASP GLN PHE GLU CYS LEU TYR PRO TYR PRO VAL HIS HIS
 SEORES
         18 A
               349
                    PRO CYS ASP ARG GLN SER GLN VAL ASP PHE ASP ASN PRO
         19 A
               349
 SEQRES
                    ASP TYR GLU ARG PHE PRO ASN PHE GLN ASN VAL VAL GLY
        20 A
               349
 SEORES
                    TYR GLU THR VAL VAL GLY PRO GLY ASP VAL LEU TYR ILE
 SEQRES
        21 A
               349
                    PRO MET TYR TRP TRP HIS HIS ILE GLU SER LEU LEU ASN
 SEQRES
        22 A
               349
               349 GLY GLY ILE THR ILE THR VAL ASN PHE TRP TYR LYS GLY
        23 A
 SEQRES
                    ALA PRO THR PRO LYS ARG ILE GLU TYR PRO LEU LYS ALA
        24 A
               349
 SEQRES
                    HIS GLN LYS VAL ALA ILE MET ARG ASN ILE GLU LYS MET
         25 A
               349
 SEORES
                    LEU GLY GLU ALA LEU GLY ASN PRO GLN GLU VAL GLY PRO
         26 A 349
 SEQRES
                     LEU LEU ASN THR MET ILE LYS GLY ARG TYR ASN
        27 A 349
 SEQRES
 HET
        FE2 A1350
                          1
 HET
        AKG
            A1351
                         10
                          5
 HET
        SO4
             A1352
       . SO4
             A1353
                          5
 HET
             A1354
 HET
        SO4
 HETNAM
             FE2 FE (II) ION
 HETNAM
            AKG 2-OXYGLUTARIC ACID
 HETNAM
             SO4 SULFATE ION
  FORMUL
           3
             FE2
                     FE1 2+
  FORMUL
           4
              AKG
                     C5 H6 O5
  FORMUL
           5
              SO4
                     3 (O4 S1 2-)
                    *3(H2 O1)
           6
  FORMUL
              НОН
               1 ASP A
                         28 LEU A
                                     32
  HELIX
           1
               2 ASP A
                             ASN A
                                     58
  HELIX
           2
                         49
                                          5
           3
               3 VAL A
                         70
                             TRP A
                                     76
  HELIX
                         77
                             ILE A
                                          1
                                      85
  HELIX
           4
               4 ASP A
                        104
                             GLN A
                                    112
           5
               5 ASP A
  HELIX
```

5

10

7

9

HELIX	6 6 PHE A 125 ARG A 138 1	Į.
HELIX	7 7 GLY A 155 GLY A 164 1	
HELIX	8 8 ASN A 166 ARG A 177 1 12	<u> </u>
HELIX	9 9 PRO A 220 ASP A 222 5	
HELIX	10 10 GLN A 223 TYR A 228 1	
HELIX	11 11 PHE A 252 VAL A 258 5	1
HELIX	12 12 LYS A 311 GLY A 331 1	
HELIX		3
HELIX	14 14 GLU A 335 LYS A 345 1	L
SHEET	1 AA 5 THR A 39 PRO A · 41 0	
SHEET	2 AA 5 GLY A 260 VAL A 265 1 O GLY A 260 N ARG A 40	
SHEET	3 AA 5 LYS A 214 PHE A 219 -1 O LYS A 214 N VAL A 265	
SHEET	4 AA 5 TRP A 278 SER A 283 -1 O TRP A 278 N PHE A 219	
SHEET	5 AA 5 VAL A 195 HIS A 199 -1 O THR A 196 N ILE A 281	•
SHEET	1 AB 6 ARG A 44 LEU A 45 0	
SHEET	2 AB 6 VAL A 62 LEU A 64 1 O VAL A 63 N LEU A 45	
SHEET	3 AB 6 VAL A 270 ILE A 273 -1 O VAL A 270 N LEU A 64	
SHEET	4 AB 6 GLN A 203 LYS A 211 -1 O ASN A 205 N ILE A 273	
SHEET	5 AB 6 THR A 290 LYS A 298 -1 O ILE A 291 N ILE A 210	
SHEET	6 AB 6 LEU A 182 SER A 184 -1 N THR A 183 O TRP A 296 1 AC 9 ARG A 44 LEU A 45 O	
SHEET SHEET		
SHEET		
SHEET	3 AC 9 VAL A 270 ILE A 273 -1 O VAL A 270 N LEU A 64. 4 AC 9 GLN A 203 LYS A 211 -1 O ASN A 205 N ILE A 273	
SHEET	5 AC 9 THR A 290 LYS A 298 -1 O ILE A 291 N ILE A 210	
SHEET	6 AC 9 LEU A 186 GLY A 190 -1 O LEU A 186 N ASN A 294	
SHEET	7 AC 9 ARG A 143 THR A 149 -1 O LEU A 146 N ILE A 189	
SHEET	8 AC 9 ASP A 89 ALA A 95 -1 O SER A 91 N GLN A 147	
SHEET	9 AC 9 SER A 118 LYS A 124 -1 O ASN A 119 N SER A 94	
LINK	FE FE2 A1350 NE2 HIS A 199 1555 1555	
LINK	FE FE2 A1350 OD2 ASP A 201 1555 1555	
LINK	FE FE2 A1350 NE2 HIS A 279 1555 1555	
LINK	FE FE2 A1350 O1 AKG A1351 1555 1555	
LINK .	FE FE2 A1350 O5 AKG A1351 1555 1555	
CISPEP	1 TYR A 308 PRO A 309 0 2.48	
SITE	1 FEA 3 HIS A 199 ASP A 201 HIS A 279	
SITE	1 AKG 13 TYR A 145 LEU A 188 THR A 196 HIS A 199	
SITE	2 AKG 13 ASP A 201 ASN A 205 PHE A 207 LYS A 214	
SITE	3 AKG 13 HIS A 279 ILE A 281 ASN A 294 TRP A 296	
SITE	4 AKG 13 HOH Z 1	
SITE	1 SA1 4 ARG A 138 GLY A 140 GLU A 141 GLU A 142	
SITE	1 SA2 ·5 ARG A 143 GLU A 192 GLY A 193 · LEU A 285	
SITE	2 SA2 5 ASN A 286	
SITE	1 SA3 4 LYS A 107 GLU A 202 ARG A 320 LYS A 324	
CRYST1	86.342 86.342 146.732 90.00 90.00 90.00 P 41 21 2 8	
ORIGX1 ORIGX2	1.000000 0.000000 0.000000	
ORIGX2	0.000000 1.000000 0.000000 0.00000 0.000000 0.000000 1.000000 0.00000	
SCALE1		
SCALE2		
SCALE3	0.000000 0.011582 0.000000 0.00000 0.000000 0.000000 0.006815 0.00000	
ATOM	1 N GLU A 15 8.558 32.684 9.824 1.00 41.85	N
ATOM	2 CA GLU A 15 7.178 32.135 9.672 1.00 42.19	N C
ATOM	3 C GLU A 15 7.180 30.645 9.998 1.00 42.19	C
ATOM	4 O GLU A 15 7.959 29.895 9.424 1.00 42.28	Ö
ATOM.	5 CB GLU A 15 6.661 32.366 8.258 1.00 42.28	C
ATOM	6 N PRO A 16 6.281 30.198 10.866 1.00 42.29	N
ATOM	7 CA PRO A 16 6.376 28.826 11.391 1.00 42.53	Č
ATOM	8 C PRO A 16 6.351 27.762 10.307 1.00 42.54	Ċ
MOTA	9 O PRO A 16 5.571 27.819 9.369 1.00 42.92	ŏ
MOTA	10 CB PRO A 16 5.172 28.713 12.337 1.00 42.63	C

MOTA	11 C	G E	PRO A	. :	16		4.749	30.155	12.612	1.00	42.41		С
ATOM	12 C	D E	PRO A	. :	16 .		5.103	30.916	11.382	1.00			C.
MOTA	13 N	1 <i>1</i>	ARG A		17		7.231	26.791	10.446	1.00	42.51		N
ATOM	. 14	CA A	ARG A		17		7.337	25.723	9.478	1.00	42.62		С
ATOM	15 0	. 1	ARG A	1	17		6.095	24.856	9.527	1.00	42.85		C
ATOM			ARG A	<i>.</i>	17		5.492	24.705	10.587	1.00	43.51		0
ATOM			ARG A		17		8.505	24.800	9.845	1.00	42.50		C
ATOM			ARG A		17		9.871	25.434	9.859	1.00	42.22		С
ATOM			ARG A		17		10.995	24.466	10.228	1.00	42.12		C
MOTA			ARG A		17		11.085	24.138	11.656	1.00	42.49		N
MOTA			ARG Z		17		11.588	24.943	12.607	1.00	42.43		С
MOTA			ARG Z		17		12.033	26.158	12.316	1.00	42.11		N
ATOM			ARG A		17		11.649	24.529	13.869	1.00	42.25		N
ATOM			GLU I		18		5.742	24.242	8.404	1.00	42.60		N
ATOM			GLU I		18		4.662	23.268	8.405				C
ATOM			GLU Z		18		5.203	21.870	8.728		41.90		С
ATOM			GLU .		18		6.249	21.472	8.216		41.98		0
ATOM			GLU .		18		3.988	23.224	7.041		42.57		С
ATOM			GLU .		18		3.363	24.537	6.620		43.60		С
ATOM			GLU		18	•	1.993	24.756	7.233		45.11		C
ATOM			GLU		18		1.365	23.766	7.686		45.48	•	0
ATOM			GLU		18		1.546	25.926	7.253	1.00	46.49		O
MOTA		N	GLU		19		4.487	21.133	9.578		41.27		N
ATOM			GLU		19		4.806	19.737	9.894		40.61		C
ATOM		C	GLU		19		4.478	18.802	8.748	1.00			c ·
MOTA		Ö	GLU		19	•	3.424	18.915	8.137	1.00			Ō
ATOM		CB	GLU		19		4.024	19.299	11.128		40.72		Ċ
ATOM		CG	GLU		19		4.507	20.034	12.361		42.24		C
ATOM	39	CD	GLU		19		4.358	19.278	13.668		44.37		Ċ
ATOM	40	OEl	GLU		19		3.852	18.127	13.680		46.17		o
ATOM	41	OE2	GLU		19		4.769	19.863	14.700		45.44		ō
ATOM	42	N	ALA		20		5.369	17.859	8.478		38.99		N
ATOM	43	CA	ALA		20		5.164	16.922	7.390		38.71		C
ATOM	44	C	ALA		20		3.831	16.232	7.542		38.51		Ċ
ATOM	45	0	ALA		20		3.391	15.933	8,649		38.80		ō
ATOM	46	СВ	ALA		20		6.280	15.895	7.328		38.51		Ċ
	47	И	GLY		21		3.180	15.991	6.419		38.03		N
ATOM ATOM	48	CA	GLY		21		1.924	15.290	6.449	1.00			C
ATOM .	49	C.	GLY		21		0.746	16.205	6.682	1.00			Ċ
ATOM	50	0	GLY		21		-0.328	15.743	7.049	1.00			ō
ATOM	51	И	ALA		22		0.941	17.497	6.447		38.40		N
ATOM	52	CA	ALA		22		-0.130	18.472	6.571		38.50		C
ATOM	53	C	ALA		22		-0.725	18.413			38.60		Ċ
ATOM	54	0	ALA		22		-1.930	18.547			38.65		Ō
ATOM	55	СВ	ALA		22		-1.196	18.242			38.61		c
ATOM	56	N	LEU		23		0.135	18.206			38.75		N
ATOM	57	CA	LEU		23		-0.297	18.257			38.82		Ç
ATOM	58	C	LEU		23		-0.321	19.684			38.78		C
ATOM	59	Ö	LEU		23		-0.525				38.74		Ō
ATOM	60	СВ	LEU		23		0.523				38.77		Ċ
ATOM	61	CG	LEU		23		0.421				39.03		Č
ATOM	62		. LEU		23		1.203				39.08		Ċ
ATOM	63		LEU		23		-1.070				39.43		č
ATOM	64	N N	GLY				-0.094				0 38.75		N
	65	CA	GLY				-0.248				0 38.79		C
MOTA MOTA	66	CA	GLY				0.972				0 38.90		Č
	67	0	GLY				2.042				0 39.06		Ö
MOTA	68	N	PRO				0.791				0 39.19		N
ATOM		CA	PRO				1.903				0 39.35		c
ATOM	69 70	CA	PRO				2.332				0 39.62		č
ATOM	70 71	0	PRO				1.492				0 39.48		Ö
MOTA	1 1	J	בתנ	, A	. 25		1.434	. 23.03					•

· ATOM	72	СВ	PRO	A	25	1.299	26.062	12.019	1.00 39.24	С
MOTA	73	CG	PRO		25	-0.142	25.920	11.961	1.00 38.71	Č
ATOM	74	CD	PRO		25	-0.490	24.616	11.365	1.00 39.17	C
ATOM	75	N	ALA		26	3.631	23.899	13.252	1.00 40.22	N
ATOM	76	CA	ALA		26	4.170	23.342	14.476	1.00 40.79	С
ATOM	77	C	ALA		26	3.930	24.294	15.666	1.00 41.07	С
ATOM	78	0	ALA		26	3.769	23.837	16.797	1.00 41.57	0
ATOM	79	CB	ALA		26	5.633	23.068	14.300	1.00 40.98	С
ATOM	80	N	TRP		27	3.931	25.605	15.429	1.00 40.80	. N
MOTA	81	CA	TRP		27	3.543	26.552	16.477	1.00 40.67	С
ATOM	82	C	TRP		27	2.982	27.848	15.880	1.00 40.33	С
ATOM ATOM	83	O	TRP		27	2.777	27.940	14.675	1.00 40.13	0
ATOM	84 85	CB CG	TRP		27	4.742	26.860	17.358	1.00 40.70	С
ATOM	86	CD1	TRP		27	5.942	27.014	16.558	1.00 41.36	С
ATOM	87	CD2	TRP TRP		27 27	6.762	26.023	16.074	1.00 43.03	С
ATOM	88	NE1			27	6.466	28.233	16.084	1.00 40.41	С
ATOM	89	CE2	TRP		27	7.788 7.618	26.579 27.938	15.344	1.00 42.65	N
ATOM	90	CE3	TRP		27	6.081	29.555	15.331	1.00 41.20	C
MOTA	91	CZ2	TRP		27	8.370	28.912	16.223 14.732	1.00 40.47	C
ATOM	92	CZ3	TRP		27	6.827	30.514	15.640	1.00 41.10 1.00 41.11	. C
ATOM	93	CH2	TRP		27	7.962	30.198	14.900	1.00 41.11	C
ATOM	94	N	ASP		28	2.677	28.830	16.723	1.00 41.57	C N
ATOM	95	CA	ASP		28	2.322	30.143	16.209	1.00 39.78	. C
ATOM	96	С	ASP		28	2.802	31.257	17.121	1.00 39.17	
MOTA	97	0	ASP	Α	28	3.227	31.013	18.240	1.00 39.00	ő
MOTA	98	CB	ASP	Α	28	0.826	30.254	15.981	1.00 40.16	C
MOTA	99	CG	ASP		28	0.066	30.380	17.258	1.00 40.79	c
MOTA	100	OD1			28	0.044	31.496	17.821	1.00 41.30	ō
MOTA	101		ASP		28	-0.531	29.414	17.774	1.00 42.25	Ō
MOTA	102	N	GLU		29	2.720	32.486	16.624	1.00 38.73	N
ATOM	103	CA	GLU		29	3.223	33.663	17.341	1.00 38.23	С
ATOM	104	C	GLU		29	2.739	33.764	18.781	1.00 37.69	C
MOTA MOTA	105 106	O CB	GLU		29	3.492	34.131	19.664	1.00 37.34	0
ATOM	107	N	GLU SER		29 30	2.834	34.924	16.594	1.00 38.20	C
MOTA	108	CA	SER		30	1.482	33.418	19.012	1.00 37.46	· N
MOTA	109	C	SER		30	0.874 1.562	33.583 32.774	20.324	1.00 37.18	C
ATOM	110	Õ	SER		30	1.282	32.774	21.399 22.577	1.00 36.93	C
ATOM	111	СВ	SER		30	-0.595	33.164	20.284	1.00 36.82 1.00 37.23	0
MOTA	112	OG	SER		30	-0.744	31.792	20.619	1.00 37.23	C 0
MOTA	113	N	GLN		31	2.441	31.867	20.999	1.00 36.85	N
ATOM	114	CA	GLN		31	3.128	31.021	21.961	1.00 36.77	C
MOTA	115	С	GLN	Α	31	4.445	31.636	22.340	1.00 36.59	Č
MOTA	116	0	GLN		31	5.141	31.127	23.220	1.00 36.74	ō
ATOM	117	CB	GLN		31	3.366	29.621	21.395	1.00 36.71	C
MOTA	118	CG	GLN		31	2.084	28.828	21.234	1.00 36.97	Ċ
MOTA	119	CD	GLN		31	2.282	27.497	20.560	1.00 36.68	C
ATOM	120		GLN		31		27.386	19.346	1.00 36.62	0
ATOM	121		GLN		31	2.601	26.478	21.343	1.00 36.85	N
ATOM ATOM	122	N	LEU		32	4.794	32.726	21.670	1.00 36.32	N
ATOM	123 124	CA	LEU		32	6.050	33.381	21.942	1.00 36.17	С
ATOM	125	С 0	LEU		32	5.817.	34.498	22.921	1.00 36.09	C
ATOM	126	CB	LEU		32 32	4.837	35.233	22.815	1.00 36.18	0
ATOM	127	CG	LEU		32	6.673 6.990	33.928	20.664	1.00 36.07	C
ATOM	128		LEU		32	7.747	32.871 33.457	19.604 18.453	1.00 36.72	C
ATOM	129		LEU		32	7.747	31.744	20.161	1.00 36.96 1.00 37.31	C
MOTA	130	N	ARG		33	6.700	34.576	23.908	1.00 37.31	C
ATOM	131	CA	ARG		33	6.713	35.671	24.851	1.00 35.99	и С
MOTA	132	С	ARG		33	7.171	36.941	24.130	1.00 35.95	C
						• -				C

ATOM	133	0	ARG Z	A.	33		7.950	36.888	23.188	1.00			0
MOTA	134	CB	ARG Z	A	33		7.671	35.350	25.991	1.00			C
MOTA	135	CG	ARG 2		33		7.210	34.204	26.854	1.00			C
MOTA	136	CD	ARG		33		8.082	33.948	28.070	1.00			С
ATOM	137	NE	ARG .		33		7.479	32.927	28.923		37.39		N
MOTA	138	CZ	ARG .		33		6.501	33.160	29.785	1.00			C
ATOM	139		ARG .		33		6.027	34.385	29.931		37.75		N N
MOTA	140		ARG .		33		6.001 6.707	32.171 38.088	30.513		38.47 35.92		N
ATOM ATOM	141 142	N CA	SER SER		34 34		7.017	39.331	24.588 23.902		36.05		C
ATOM	143	CA	SER		34		8.044	40.146	24.671		35.47		C
ATOM	144	0	SER		34		7.940	40.311	25.884		35.41		Ö
ATOM	145	СВ	SER		34		5.732	40.120	23.691		36.27		Ċ
ATOM	146	OG	SER		34		5.046	40.253	24.920		37.99		0
ATOM	147	N	TYR		35		9.031	40.655	23.945		35.01		N
ATOM	148	CA	TYR		35	;	10.140	41.370	24.543	1.00	34.69		С
ATOM	149	С	TYR	Α	35		10.400	42.693	23.853	1.00	34.59		С
MOTA	150	0	TYR	A	35		9.841	42.989	22.813	1.00	34.45		0
MOTA	151	CB	TYR	A	35		11.384	40.501	24.469		34.71		С
ATOM	152	CG	TYR	A	35		11.228	39.222	25.232		34.43		С
MOTA	153	CD1			35		10.928	39.246	26.573		33.87		С
MOTA	154	CD2			35		11.350	37.986	24.602		35.32		C
ATOM	155	CE1			35		10.775	38.087	27.285		34.96		C
ATOM	156	CE2			35		11.192	36.807	25.309		35.50		C
MOTA	157	CZ	TYR		35		10.904	36.865	26.653		35.16	•	С 0
ATOM	158	OH	TYR		35		10.742	35.709	27.376		34.77		Ŋ
ATOM	159	N	SER		36 36		11.290 11.572	43.481 44.814	24.429 23.924		34.77 34.74		C
MOTA MOTA	160 161	CA C	SER SER		36 36		12.567	44.926	22.771		34.30		C
MOTA	162	o	SER		36		12.805	46.011	22.287	1.00			ŏ
MOTA	163	СВ	SER		36		12.127	45.627	25.077		34.91		Ċ
ATOM	164	OG	SER		36		13.395	45.116	25.449	1.00			Ō
ATOM	165	N	PHE		37		13.155	43.838	22.318		34.15		N
MOTA	166	CA	PHE		37		14.193	43.963	21.306		34.11		С
ATOM	167	С	PHE		37		13.969	43.177	20.044	1.00	34.07		С
ATOM	168	0	PHE	A	37		13.356	42.109	20.017	1.00	33.98	•	0
MOTA	169	CB	PHE	Α	37		15.514	43.479	21.867		34.08		С
MOTA	170	CG	PHE		37		15.417	42.147	22.438		34.33		C
MOTA	171		L PHE		37		15.445	41.034	21.621		35.66		C
MOTA	172		2 PHE		37		15.208	41.990	23.777		35.42		C
ATOM	173		l PHE		37		15.320	39.782	22.143		35.73		C
ATOM	174		2 PHE		37		15.084	40.736	24.317		36.14		C C
MOTA	175		PHE		37		15.141 14.565	39.628 43.682	23.497 18.991		36.55		N
ATOM ATOM	176 177		PRO PRO		38 38		14.474	43.028			33.91		C
ATOM	178		PRO		38		15.445	41.878	17.640		33.74		Ċ
ATOM	179		PRC		38		16.366	41.803	18.441		33.82		Ö
ATOM	180				38		14.887	44.133			34.03		Ċ
ATOM	181						15.874	44.935			33.99		С
ATOM	182						15.385	44.903			33.80		С
ATOM	183		THE				15.233				34.02		N
ATOM	184						16.089			1.00	34.00		C
ATOM	185	C	THE	RA	39		16.035	39.490	15.008	1.00	34.09		С
MOTA	186		THE				15.137				34.05		0
MOTA	187						15.563				33.94		C
MOTA	· 188						14.250				34.18		0
MOTA	189		2 THE				15.338				34.09		C
MOTA	190		ARC				16.992				34.62		N
ATOM	191						17.066				35.13		C
MOTA	192		ARG	j A G A			17.100 17.419				0 35.17 0 34.96		0
MQTA	193	3 0	MA	J A	. 410		11.413	20.103	74.474	1.00	. 34.30		9

AT	OM	194	CB	ARG	A	40	18.352	38.649	12.568	1 00	35.54		_
AT	ОМ	195	CG	ARG		40	18.358	40.103					C
AT		196	CD	ARG		40			12.287		38.87		С
							16.975	40.597	11.893		42.88		С
AT		197	NE	ARG		40	16.737	40.908	10.489	1.00	44.50		N
AT		198	CZ	ARG	A	40	15.554	41.298	10.076	1.00	46.73		С
AT	OM	199	NH1	ARG	A	40	14.574	41.350	10.974		46.73		N
AT	OM	200	NH2	ARG	Α	40	15.334	41.636	8.802		48.87		
AT	OM	201	N	PRO		41	16.775						N
AT		202	CA					36.026	12.285		35.20		N
				PRO		41	16.749	34.579	12.348		35.24		С
AT		203	С	PRO		41	18.114	33.973	12.275	1.00	35.10		С
AT		204	0	PRO	Α	41	18.995	34.455	11.573		35.96		ō
AT	OM	205	CB	PRO	A	41	16.003	34.208	11.079		35.27		c
AT	OM	206	CG	PRO	A	41	15.408	35.453	10.640		34.93		
AT	OM	207	CD	PRO		41	16.381	36.494					C
AT		208	N	ILE		42 .			10.953		34.81		С
AT							18.277	32.910	13.022		34.55		N
		209	CA	ILE		42	19.435	32.099	12.909	1.00	34.29		С
AT		210	С	ILE		42	19.145	31.194	11.713	1.00	34.29		С
AT	OM	211	0	ILE	A	42	18.035	30.654	11.598		34.38		ō
AT	OM	212	CB	ILE	A	42	19.545	31.258	14.150		34.14		
AT	OM	213	CG1	ILE		42	19.742	32.152.	15.368			•	C
AT		214	CG2	ILE		42					34.83		С
AT							20.679	30.297	14.016		34.41		С
			.CD1			42	19.479	31.467	16.678	1.00	35.37	•	Ç
AT		216	N	PRO		43	20.127	31.010	10.836	1.00	33.80		N
AT		217	CA	PRO	A	43	19.982	30.122	9.686		33.62		C
AT	OM	218	С	PRO	A	43	19.714	28.676	10.066		33.65		C
AT	OM	219	0	PRO	Α	43	20.320	28.198	11.015		33.60		
AT	OM	220	CB	PRO		43	21.366						0
AT		221	CG	PRO		43		30.174	9.043		33.63		С
AT							21.986	31.385	9.543		33.11		C
		222	CD	PRO		43	21.455	31.630	10.882	1.00	33.51		С
AT		223	N	ARG		44	18.820	28.007	9.341	1.00	33.86		N
AT		224	CA	ARG	Α	44	18.597	26.572	9.486		34.00		C
AT	MO	225	C	ARG	A	44	19.176	25.968	8.247		33.87		
AT	OM	226	0	ARG		44	18.783	26.319					C
AT	OM	227	СВ	ARG		44			7.152		33.76	•	0
AT		228	CG ·	ARG			17.125	26.185	9.520		34.10		С
						44	16.301	26.879	10.577		35.44		С
AT	•	229	CD	ARG		44	14.781	26.505	10.583	1.00	37.36		С
AT		230	NE	ARG		44	14.415	25.108	10.265	1.00	37.59		N
AT		231	CZ	ARG	A	44	14.237	24.144	11.187		39.71		C
AT	OM	232	NH1	ARG	Α	44	14.429	24.396	12.487		39.94		
AT	OM	233	NH2	ARG		44	13.876	22.915					N
AT	ОМ	234	N	LEU		45	20.086		10.821		40.07		N
AT		235	CA					25.030			33.98		N
AT	,			LEU		45	20.747	24.467	7.269		34.15		C
		236	С	LEU		45	20.950	22.995	7.389	1.00	34.37		С
AT		237	0	LEU		45	20.901	22.453	8.486	1.00	34.52		0
AT		238	CB	LEU	A	45	22.116	25.090	7.183		34.25		C
ATO	OM	239	CG	LEU	Α	45	22.080	26.576	6.905		34.80		
AT	OM	240	CD1	LEU		45	23.454	27.095				_	C
ATO		241		LEU		45			7.177		36.05	Ť	С
AT		242					21.655	26.837	5.481		34.78		С
			N	SER		46	21.199	22.343	6.255	1.00	34.55		N
AT		243	CA	SER		46	21.549	20.949	6.306	1.00	34.60		C
ATO		244	C	SER	Α	46	22.985	20.838	6.681		34.89		Č
ATO	OM	245	0	SER	A	46	23.826	21.671	6.383		34.54		
ATO	MO	246	CB	SER		46	21.356	20.206					0
ATO		247	OG	SER		46			5.006		34.64		С
	OM .	248	N				22.231	19.090	4.989		33.61		0
				GLN		47	23.247	19.736	7.324	1.00	35.61		N
ATO		249	CA	GLN		47	24.539	19.462	7.866		36.10		C
ATO		250	С	GLN		47	25.565	19.368	6.746		35.96		c
ATO		251	0	GLN	A	47	26.754	19.537	6.969		36.13		
ATO	MO	252	СВ	GLN		47	24.399	18.168	8.669		36.22		0
ATO		253	CG	GLN		47	25.604						C
ATO		254	CD	GLN		47		17.340	8.730		37.25		С
`				CHIM	1.7	31	25.724	16.459	7.532	1.00	39.03		С

										_
ATOM.	255	OE1	GLN A	A.	47	24.766	16.306	6.759	1.00 38.79	0
MOTA	256	NE2	GLN A	A	47	26,902	15.872	7.354	1.00 41.44	N
MOTA	257		SER A		48	25.088	19.146	5.531	1.00 35.87	N
								4.391		· C
MOTA	258		SER A		48	25.958	18.938		1.00 35.90	
MOTA	259	С	SER I		48	26.301	20.244	3.715	1.00 36.06	С
ATOM	260	0	SER A	A.	48	·27.215	20.334	2.897	1.00 35.95	0
ATOM	261	CB	SER A	A	48	25.214	18.073	3.402	1.00 35.97	C.
ATOM	262	OG	SER I		48	23.933	18.635	3.158	1.00 36.62	0
	263						21.266	4.075		
ATOM		N	ASP 2		49	25.552			1.00 36.34	N
ATOM	264	CA	ASP .		49	25.701	22.564	3.491	1.00 36.65	С
ATOM	265	С	ASP .	A	49	26.963	23.236	3.952	1.00 37.06	C
ATOM	266	0	ASP .	Α	49	27.114	23.507	5.138	1.00 37.24	0
ATOM	267	CB	ASP .		49	24.545	23.405	3.953	1.00 36.80	С
ATOM	268	CG	ASP		49	24.441	24.674	3.206	1.00 37.08	Ċ
ATOM	269		ASP		49	25.490	25.217	2.810	1.00 37.38	0
MOTA	27.0	OD2	ASP .		49	23.343	25.187	2.953	1.00 38.64	0
MOTA	271	N	PRO	A	50	27.857	23.565	3.029	1.00 37.42	N
ATOM	272	CA	PRO	Α	50	29.113	24.196	3.430	1.00 37.32	С
MOTA	273	C	PRO		50	28.881	25.413	4.298	1.00 37.46	· C
ATOM	274	ō	PRO		50	29.742	25.727	5.113	1.00 37.85	0
MOTA	275	CB	PRO		50	29.750	24.604	2.108	1.00 37.21	С
ATOM	276	CG	PRO		50	29.134	23.726	1.086	1.00 37.39	C
MOTA	277	CD	PRO	Α	50	27.755	23.395	1.568	1.00 37.34	С
ATOM	278	N ·	ARG	A	51	27.743	26.081	4.162	1.00 37.64	N
ATOM	279	CA	ARG		51	27.535	27.301	4.932	1.00 38.06	С
ATOM	280	C	ARG		51	27.470	27.000	6.421	1.00 38.26	Č
ATOM		Õ	ARG		51	27.920		7.250	1.00 38.47	ō
	281						27.798			
MOTA	282	CB	ARG		51	26.282	28.055	4.470	1.00 38.14	С
ATOM	283	CG	ARG		51	26.418	28.692	3:059	1.00 38.89	С
ATOM	284	CD	ARG	A	51	25.117	29.259	2.455	1.00 39.65	С
ATOM	285	NE	ARG	Α	51	24.121	28.211	2.175	1.00 41.25	N
MOTA	286	CZ	ARG		51	22.798	28.404	2.078	1.00 41.86	С
ATOM	287		ARG		51	22.264		2.225	1.00 43.70	N
ATOM	288		ARG		51				•	
						21.994	27.393	1.818	1.00 41.90	N
ATOM	289	N	ALA		52	26.936		6.770	1.00 38.26	N
ATOM	290	CA	ALA		52	26.807		8.171	1.00 38.30	С
MOTA	291	С	ALA	Α	52	28.206	25.374	8.683	1.00 38.45	С
ATOM	292	0	ALA	Α	52	28.572	25.922	9.732	1.00 38.37	0
MOTA	293	CB	ALA	Α	52	26.085		8.344	1.00 38.25	С
MOTA	294	N	GLU		53	. 29.003		7.901	1.00 38.56	N
ATOM	295	CA	GLU		53	30.361		8.291	1.00 38.94	C
ATOM	296	C	GLU		53	31.145				C
ATOM	297	0	GLU		53	31.970		9.386	1.00 38.49	0
ATOM	298	CB	GLU	Α	53	31.060	23.507	7.314	1.00 38.91	C
MOTA	299	CG	GLU	Α	53	32.139	22.738	8.035	1.00 40.55	C
MOTA	300	CD	GLU	Α	53	31.662		8.579	1.00 42.38	С
MOTA	301		GLU		53	30.475		8.957	1.00 43.42	ō
ATOM	302		GLU		53	32.498		8.639	1.00 44.15	ő
MOTA	303	N	GLU		54	30.897		7.662	1.00 39.21	N
MOTA	304	CA	GLU			31.592	28.004	7.870	1.00 39.44	С
ATOM	305	С	GLU	Α	54	31.092	28.625	9.144	1.00 39.05	С
ATOM	306	0	GLU	Α	54	31.848	29.262	9.869	1.00 39.51	0
ATOM	307	СВ	GLU		54	31.337		6.772	1.00 39.59	C
MOTA	308	CG	GLU		54	31.940		5.433	1.00 33.33	C
ATOM	309	CD	GLU		54	31.098		4.302	1.00 44.74	C
ATOM	310		L GLU		54	30.546		4.509	1.00 46.67	0
MOTA	311		GLU		54	30.972		3.234	1.00 44.49	0
MOTA	312	N	LEU	Α	55	29.812	28.468	9.424	1.00 38.37	N
MOTA	313	CA	LEU			29.291		10.583		С
ATOM	314	C	LEU			29.906		11.847		C
ATOM	315	ō	LEU			30.359		12.693		ō
	720	•		••	-	50.55		00	2.00 37.03	Ū

MOTA	316	CB	LEU	Α	55	27.789	29.006	10.648	1.00 38	.28	•	С
ATOM	317	CG	LEU	Α	55	27.142	29.846	9.564	1.00 37			Č
ATOM	318	CD1	LEU	Α	55	25.722	29.443	9.409	1.00 38			Ċ
ATOM	319		LEU		55	27.233	31.279	9.951	1.00 37			C
ATOM	320	N	ILE		56	29.938	27.286	11.971	1.00 37			N
ATOM	321	CA	ILE		56	30.455	26.667	13.183	1.00 37		-	C
MOTA	322	C	ILE		56	31.912	26.988	13.321	1.00 37			
ATOM	323	ō	ILE		56	32.373	27.320	14.406	1.00 37			C
MCTA	324	СВ	ILE		56	30.288	25.171					0
ATOM	325	CG1			56	28.810	24.789	13.175	1.00 37			C
ATOM	326	CG2			56	30.968		13.213	1.00 36			C
ATOM	327		ILE				24.602	14.397	1.00 37			С
ATOM	328	N			56	28.543	23.358	12.820	1.00 36			С
ATOM	329	CA	GLU GLU		57 57	32.627	26.899	12.204	1.00 37			N
ATOM	330	•				34.045	27.204	12.166	1.00 38			C
ATOM		C	GLU		57 57	34.277	28.569	12.784	1.00 38			C
	331	0	GLU		57	35.210	28.758	13.566	1.00 38			0
ATOM	332	CB	GLU		57	34.547	27.214	10.725	1.00 38			C
MOTA	333	CG	GLU		57	36.038	27.461	10.559	1.00 40			C
ATOM	334	CD	GLU		57	36.870	26.539	11.424	1.00 42			С
ATOM	335		GLU		57	36.527	25.329	11.487	1.00 43			0
ATOM	336	OE2			57	37.852	27.032	12.044	1.00 44			0
MOTA	337	N.	ASN		58	33.394	29.508	12.460	1.00 38			N
MOTA	338	CA	ASN		58	33.546	30.890	12.891	1.00 38			С
ATOM	339	C	ASN		58	32.849	31.221	14.167	1.00 38			С
MOTA	340	0	ASN		58 .	32.683	32.387	14.507	1.00 37			0
MOTA	341	CB	ASN		58	32.955	31.813	11.853	1.00 38	3.73		С
ATOM	342	CG	ASN		58	33.991	32.455	11.013	1.00 39	9.49		С
ATOM	343		ASN		58	34.501	31.841	10.083	1.00 42	2.51		0
ATOM	344	ND2	ASN		58	34.322	33.704	11.324	1.00 40	0.15		N
MOTA	345	N	GLU	Α	59	32.399	30.196	14.856	1.00 37	7.88		N
ATOM	346	CA	GLU		59	31.683	30.396	16.092	1.00 37	7.68		С
ATOM	347	С	GLU	Α	59	30.479	31.307	16.005	1.00 37	7.57		С
ATOM	348	0	GLU	Α	59	30.305	32.203	16.813	1.00 36	6.94		0
ATOM	349	CB	GLU	A	59	32.663	30.857	17.118	1.00 37	7.60		C
MOTA	350	CG	GLU	A	59	33.710	29.785	17.212	1.00 38	3.25		С
ATOM	351	CD	GLU	A	59	34.545	29.886	18.435	1.00 38	8.10		С
MOTA	352	OE1			59	35.654	30.430	18.303	1.00 40	0.30		0
ATOM	353	OE2	GLU	A	59	34.089	29.420	19.498	1.00 37	7.62		0
MOTA	354	N	GĽÜ	Α	60	29.630	31.025	15.025	1.00 37	7.73		N
MOTA	355	CA	GLU	A	60	28.347	31.692	14.902	1.00 37	7.79		C
ATOM	356	С	GLU		60	27.290	30.620	14.923	1.00 37	7.12		С
MOTA	357	0	GLU	A	60	27.488	29.539	14.388	1.00 37			0
ATOM	358	CB	GLU	Α	60	28.252	32.456	13.606	1.00 38			С
MOTA	359	CG	GLU		60	29.388	33.411	13.414	1.00 39			С
MOTA	360		GLU		60	28.986	34.547	12.518	1.00 42			С
MOTA	361		GLU		60	29.023	34.389	11.276	1.00 42	2.22		0
ATOM	362	OE2	GLU	A	60	28.611	35.601	13.082	1.00 46			Ō
ATOM	363	N	PRO	Α	61	26.158	30.917	15.517	1.00 3			N
ATOM	364	CA	PRO	Α	61 [']	25.111	29.919	15.680	1.00 3			C
ATOM	365	С	PRO	Α	61	24.522	29.448	14.373	1.00 3			C
ATOM	366	0	PRO	Α	61	24.534	30.159	13.386	1.00 3			0
ATOM	367	CB	PRO	A	61	24.021	30.672	16.442	1.00 3			C
MOTA	368	CG	PRO		61	24.367	32.117	16.353	1.00 3			Ċ
MOTA	369	CD	PRO		61	25.790	32.228	16.061	1.00 3			c
ATOM	370	N	VAL		62	23.981	28.247	14.380 ⁻	1.00 3			N
ATOM	371	CA	VAL		62	23.291	27.722	13.228	1.00 3			C
ATOM	372	C	VAL		62	22.438	26.584	13.720	1.00 34			c
ATOM	373	Ö	VAL		62	22.807	25.885	14.658	1.00 34			Ö
MOTA	374	СВ	VAL		62	24.237	27.189	12.156	1.00 3			C
ATOM	375		VAL		62	25.108	26.062	12.695	1.00 34			c
ATOM	376		VAL		62	23.440	26.693	10.996	1.00 3			C
	_				-			_5.550				•

ATOM 377 N VAL A 63 21.272 26.418 33.138 1.00 34.58 N ATOM 378 C A VAL A 63 20.454 25.273 13.477 1.00 33.65 C ATOM 380 O VAL A 63 20.456 24.230 12.372 1.00 33.85 C ATOM 380 O VAL A 63 20.466 24.230 12.372 1.00 33.85 C ATOM 381 CB VAL A 63 18.980 25.622 13.523 1.00 34.05 C ATOM 382 CG1 VAL A 63 18.980 25.622 13.523 1.00 34.05 C ATOM 383 CG2 VAL A 63 18.977 26.502 14.710 1.00 33.51 C ATOM 384 N LEU A 64 21.040 23.028 12.769 1.00 33.51 C ATOM 385 CA LEU A 64 21.040 21.942 11.814 1.00 34.03 C ATOM 386 C LEU A 64 19.366 20.1956 12.932 1.00 34.18 C ATOM 385 CA LEU A 64 19.366 20.1956 12.932 1.00 34.18 C ATOM 385 C A LEU A 64 19.366 20.1956 12.932 1.00 34.18 C ATOM 385 C A LEU A 64 19.366 20.956 12.932 1.00 34.18 C ATOM 389 C B LEU A 64 19.366 20.956 12.932 1.00 34.18 C ATOM 389 C B LEU A 64 19.366 20.956 12.932 1.00 34.18 C ATOM 389 C B LEU A 64 23.667 21.978 12.155 1.00 34.85 C ATOM 389 CD LEU A 64 23.667 21.978 12.155 1.00 34.85 C ATOM 391 CDL LEU A 64 23.667 21.978 12.155 1.00 34.85 C ATOM 393 CA THR A 65 18.03 20.877 1.00 14 1.00 33.36 N ATOM 393 CA THR A 65 18.035 20.177 10.704 1.00 33.36 N ATOM 394 C THR A 65 18.035 20.177 10.704 1.00 33.24 C ATOM 395 C THR A 65 17.096 18.016 10.715 1.00 32.11 C ATOM 395 C THR A 65 17.096 18.016 10.715 1.00 32.11 C ATOM 395 C THR A 65 17.858 20.540 8.320 1.00 33.15 C ATOM 395 C THR A 65 17.858 20.540 8.320 1.00 33.15 C ATOM 396 C THR A 65 17.858 20.540 8.320 1.00 33.15 C ATOM 396 C THR A 65 17.858 20.540 8.320 1.00 33.15 C ATOM 397 C THR A 65 17.858 20.540 8.320 1.00 33.15 C ATOM 398 C THR A 65 17.858 20.540 8.320 1.00 33.15 C ATOM 398 C THR A 65 17.858 20.540 8.320 1.00 33.15 C ATOM 398 C C THR A 65 17.858 20.540 8.320 1.00 33.15 C ATOM 398 C C THR A 65 17.858 20.540 8.320 1.00 33.15 C ATOM 398 C C THR A 67 22.286 18.173 10.00 10.00 33.55 C ATOM 398 C C THR A 67 22.286 18.173 10.00 10.00 33.55 C ATOM 398 C C THR A 67 22.286 18.173 10.00 33.55 C C ATOM 398 C C THR A 67 22.286 18.173 10.00 33.55 C C ATOM 398 C C THR A 67 22.286 18.173 10.00 33.55 C C ATOM 398 C C THR A 67 22.286										
ATOM 360 C VAL A 63 20.466 24.220 12.372 1.00 33.85 C C ATOM 381 CB VAL A 63 18.960 25.622 13.523 1.00 34.05 C C ATOM 382 CG1 VAL A 63 18.167 26.34349 13.523 1.00 34.05 C C ATOM 383 CG2 VAL A 63 18.167 26.520 14.710 1.00 33.51 C C ATOM 384 N LEU A 64 21.048 23.028 12.769 1.00 33.87 N ATOM 385 C LEU A 64 21.204 21.942 11.814 1.00 34.03 C C ATOM 385 C LEU A 64 21.204 21.942 11.814 1.00 34.03 C C ATOM 387 O LEU A 64 19.894 21.193 11.865 1.00 33.70 C C ATOM 389 C LEU A 64 19.894 21.193 11.865 1.00 33.70 C C ATOM 389 C LEU A 64 19.894 21.193 11.865 1.00 33.70 C C ATOM 389 C LEU A 64 19.894 21.193 11.814 1.00 34.03 C C ATOM 389 C C LEU A 64 19.894 21.193 11.814 1.00 34.03 C C ATOM 389 C C LEU A 64 22.417 21.071 12.164 1.00 33.90 C C ATOM 389 C C LEU A 64 23.667 21.978 12.155 1.00 34.18 C C ATOM 399 C C LEU A 64 23.667 21.978 12.155 1.00 34.95 C C ATOM 391 C C LEU A 64 23.667 21.978 12.155 1.00 33.90 C C ATOM 392 C T ATA 65 19.314 20.887 10.704 1.00 33.36 N ATOM 393 C D THR A 65 18.035 20.177 10.704 1.00 33.36 N ATOM 393 C T ATR A 65 18.035 20.177 10.704 1.00 33.34 C C ATOM 395 C T ATA 65 18.105 18.663 10.517 1.00 32.87 C ATOM 395 C T ATA 65 18.105 18.663 10.517 1.00 32.87 C ATOM 395 C T ATA 65 18.105 18.663 10.517 1.00 32.81 C ATOM 395 C T ATA 66 17.149 20.657 9.562 1.00 33.35 C ATOM 395 C B ATA 66 17.49 20.657 9.562 1.00 33.35 C ATOM 395 C B ATA 66 17.49 20.657 9.562 1.00 33.35 C ATOM 395 C B ATA 66 19.392 16.676 9.724 1.00 33.35 C ATOM 400 C A ASP A 66 19.392 16.676 9.724 1.00 33.55 C ATOM 401 C ASP A 66 19.392 16.676 9.744 10.00 33.55 C ATOM 401 C ASP A 66 19.392 16.676 9.744 10.00 33.55 C ATOM 402 C ASP A 66 19.392 16.676 9.744 10.00 33.55 C ATOM 402 C ASP A 66 19.392 16.676 9.744 10.00 33.55 C ATOM 401 C ASP A 66 19.392 16.676 9.744 10.00 33.55 C ATOM 402 C ASP A 66 20.629 16.019 10.199 10.00 33.55 C ATOM 402 C ASP A 66 20.587 17.484 17.588 10.00 33.55 C ATOM 401 C ASP A 66 20.587 A 66 20.587 A 66 20.587 A 66 20.587 A 66 20.587 A 66 20.587 A 66 20.587 A 66 20.587 A 66 20.587 A 66 20.587 A 66 20.587 A 66 20.587 A	MOTA	377	N	VAL A	63	21.271	26.418	13.118	1.00 34.54	N
ATOM 360 C VAL A 63 20.466 24.220 12.372 1.00 33.85 C C ATOM 381 CB VAL A 63 18.960 25.622 13.523 1.00 34.05 C C ATOM 382 CG1 VAL A 63 18.167 26.34349 13.523 1.00 34.05 C C ATOM 383 CG2 VAL A 63 18.167 26.520 14.710 1.00 33.51 C C ATOM 384 N LEU A 64 21.048 23.028 12.769 1.00 33.87 N ATOM 385 C LEU A 64 21.204 21.942 11.814 1.00 34.03 C C ATOM 385 C LEU A 64 21.204 21.942 11.814 1.00 34.03 C C ATOM 387 O LEU A 64 19.894 21.193 11.865 1.00 33.70 C C ATOM 389 C LEU A 64 19.894 21.193 11.865 1.00 33.70 C C ATOM 389 C LEU A 64 19.894 21.193 11.865 1.00 33.70 C C ATOM 389 C LEU A 64 19.894 21.193 11.814 1.00 34.03 C C ATOM 389 C C LEU A 64 19.894 21.193 11.814 1.00 34.03 C C ATOM 389 C C LEU A 64 22.417 21.071 12.164 1.00 33.90 C C ATOM 389 C C LEU A 64 23.667 21.978 12.155 1.00 34.18 C C ATOM 399 C C LEU A 64 23.667 21.978 12.155 1.00 34.95 C C ATOM 391 C C LEU A 64 23.667 21.978 12.155 1.00 33.90 C C ATOM 392 C T ATA 65 19.314 20.887 10.704 1.00 33.36 N ATOM 393 C D THR A 65 18.035 20.177 10.704 1.00 33.36 N ATOM 393 C T ATR A 65 18.035 20.177 10.704 1.00 33.34 C C ATOM 395 C T ATA 65 18.105 18.663 10.517 1.00 32.87 C ATOM 395 C T ATA 65 18.105 18.663 10.517 1.00 32.87 C ATOM 395 C T ATA 65 18.105 18.663 10.517 1.00 32.81 C ATOM 395 C T ATA 66 17.149 20.657 9.562 1.00 33.35 C ATOM 395 C B ATA 66 17.49 20.657 9.562 1.00 33.35 C ATOM 395 C B ATA 66 17.49 20.657 9.562 1.00 33.35 C ATOM 395 C B ATA 66 19.392 16.676 9.724 1.00 33.35 C ATOM 400 C A ASP A 66 19.392 16.676 9.724 1.00 33.55 C ATOM 401 C ASP A 66 19.392 16.676 9.744 10.00 33.55 C ATOM 401 C ASP A 66 19.392 16.676 9.744 10.00 33.55 C ATOM 402 C ASP A 66 19.392 16.676 9.744 10.00 33.55 C ATOM 402 C ASP A 66 19.392 16.676 9.744 10.00 33.55 C ATOM 401 C ASP A 66 19.392 16.676 9.744 10.00 33.55 C ATOM 402 C ASP A 66 20.629 16.019 10.199 10.00 33.55 C ATOM 402 C ASP A 66 20.587 17.484 17.588 10.00 33.55 C ATOM 401 C ASP A 66 20.587 A 66 20.587 A 66 20.587 A 66 20.587 A 66 20.587 A 66 20.587 A 66 20.587 A 66 20.587 A 66 20.587 A 66 20.587 A 66 20.587 A 66 20.587 A	MOTA			VAL A	63				1.00 34.18	С
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ATOM 401 C ASP A 66 19.392 16.767 9.724 1.00 33.53 C ATOM 401 C ASP A 66 20.629 16.019 10.189 1.00 33.55 C ATOM 402 O ASP A 66 21.136 15.179 9.458 1.00 33.68 O ATOM 403 CB ASP A 66 19.339 16.653 8.192 1.00 33.55 C ATOM 404 CG ASP A 66 20.397 17.484 7.508 1.00 33.55 C ATOM 405 ODI ASP A 66 20.397 17.484 7.508 1.00 35.03 O ATOM 406 ODZ ASP A 66 21.124 18.232 8.188 1.00 35.03 O ATOM 406 ODZ ASP A 66 20.583 17.456 6.284 1.00 35.31 O ATOM 407 N THR A 67 21.107 16.264 11.397 1.00 33.83 N ATOM 408 CA THR A 67 22.286 15.540 11.845 1.00 33.70 C ATOM 409 C THR A 67 22.286 15.540 11.845 1.00 33.70 C ATOM 410 O THR A 67 22.898 13.340 12.431 1.00 34.42 O ATOM 411 CB THR A 67 22.951 16.215 13.020 1.00 33.66 C ATOM 411 CB THR A 67 22.951 16.215 13.020 1.00 33.66 C ATOM 412 OG1 THR A 67 22.951 16.215 13.020 1.00 33.66 C ATOM 413 CG2 THR A 67 22.981 16.451 14.046 1.00 33.90 O ATOM 414 N ASN A 68 20.686 13.954 12.719 1.00 34.00 N ATOM 415 CA ASN A 68 20.320 12.676 13.312 1.00 34.00 N ATOM 416 C ASN A 68 20.320 12.676 13.312 1.00 34.00 N ATOM 417 O ASN A 68 21.108 12.454 14.575 1.00 33.97 C ATOM 418 CB ASN A 68 20.653 11.531 12.375 1.00 34.26 C ATOM 419 CG ASN A 68 21.108 11.531 12.375 1.00 34.26 C ATOM 420 OD1 ASN A 68 21.108 11.531 12.375 1.00 34.15 C ATOM 420 OD1 ASN A 68 21.281 11.330 15.008 1.00 33.83 O ATOM 420 OD1 ASN A 68 19.685 11.411 11.239 1.00 34.12 N ATOM 422 N LEU A 69 22.538 11.531 12.375 1.00 34.12 N ATOM 422 C LEU A 69 22.538 11.531 15.162 1.00 34.19 C ATOM 424 C LEU A 69 22.538 11.531 15.162 1.00 34.19 C ATOM 426 CB LEU A 69 22.538 11.531 15.162 1.00 34.19 C ATOM 429 CD2 LEU A 69 22.538 11.531 15.162 1.00 34.19 C ATOM 429 CD2 LEU A 69 22.538 11.531 15.162 1.00 34.19 C ATOM 429 CD2 LEU A 69 22.538 11.531 15.162 1.00 34.19 C ATOM 429 CD2 LEU A 69 22.538 11.531 15.162 1.00 34.19 C ATOM 426 CB LEU A 69 22.538 11.531 15.162 1.00 34.19 C ATOM 427 CG LEU A 69 22.538 11.531 15.321 1.00 34.10 C ATOM 428 CD1 LEU A 69 22.538 11.531 15.321 1.00 34.10 C ATOM 428 CD1 LEU A 69 22.538 11.531 15.228 1.00 34.15 N ATOM 429 CD2 LEU	ATOM	398	CG2			16.843	22.093	9.693	1.00 33.51	· C .
ATOM 401 C ASP A 66 20.629 16.0.19 10.189 1.00 33.55 C ATOM 402 O ASP A 66 21.136 15.179 9.458 1.00 33.68 O ATOM 403 CB ASP A 66 21.136 15.179 9.458 1.00 33.68 O ATOM 404 CG ASP A 66 20.397 17.484 7.508 1.00 34.00 C ATOM 405 OD1 ASP A 66 20.397 17.484 7.508 1.00 34.00 C ATOM 406 OD2 ASP A 66 20.583 17.456 6.284 1.00 35.31 O ATOM 407 N THR A 67 21.107 16.264 11.397 1.00 33.83 N ATOM 408 CA THR A 67 22.286 15.540 11.845 1.00 33.70 C ATOM 409 C THR A 67 22.286 15.540 11.845 1.00 33.83 N ATOM 409 C THR A 67 22.286 15.540 11.845 1.00 33.84 C ATOM 410 O THR A 67 22.981 16.215 13.020 1.00 33.86 C ATOM 411 CB THR A 67 22.981 16.215 13.020 1.00 33.66 C ATOM 412 CG THR A 67 23.472 17.562 12.674 1.00 33.56 C ATOM 413 CG2 THR A 67 23.472 17.562 12.674 1.00 33.56 C ATOM 414 N ASN A 68 20.686 13.954 12.719 1.00 34.10 N ATOM 415 CA ASN A 68 20.320 12.676 13.312 1.00 34.15 C ATOM 416 C ASN A 68 20.281 12.395 1.00 33.83 O ATOM 416 C ASN A 68 21.108 12.454 14.575 1.00 33.97 C ATOM 416 C ASN A 68 21.281 11.330 15.008 1.00 33.83 O ATOM 417 O ASN A 68 20.686 13.954 12.719 1.00 34.00 N ATOM 418 CB ASN A 68 21.108 12.454 14.575 1.00 34.26 C ATOM 419 CG ASN A 68 19.685 11.411 11.239 1.00 34.26 C ATOM 420 OD1 ASN A 68 19.685 11.411 11.239 1.00 34.26 C ATOM 420 OD1 ASN A 68 18.512 11.104 11.434 1.00 35.89 O ATOM 421 ND2 ASN A 68 19.685 11.411 11.239 1.00 34.15 C ATOM 422 N LEU A 69 22.486 13.419 16.334 1.00 34.12 N ATOM 423 CA LEU A 69 22.486 13.419 16.334 1.00 34.12 N ATOM 424 C LEU A 69 22.538 11.737 18.039 1.00 34.12 N ATOM 425 O LEU A 69 22.538 11.737 18.039 1.00 34.15 C ATOM 428 CD1 LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 429 CD2 LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 429 CD2 LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 429 CD2 LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 428 CD1 LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 429 CD2 LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 429 CD2 LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 433 CA VAL A 70 19.877 12.023 18.865 1.00 34.46 C ATOM 433 CA VAL A 70 19	MOTA	399	N	ASP A	66	19.265	18.173		1.00 33.09	
ATOM 402 O ASP A 66	MOTA	400	CA	ASP A	66	19.392		9.724	1.00 33.53	
ATOM	ATOM	401	С	ASP A	66	20.629	16.019	10.189	1.00 33.55	C
ATOM	ATOM	402	0	ASP A	. 66	21.136	15.179	9.458	1.00 33.68	0
ATOM 405 OD1 ASP A 66 21.124 18.232 8.188 1.00 35.03 O ATOM 406 OD2 ASP A 66 20.583 17.456 6.284 1.00 35.31 O ATOM 407 N THR A 67 21.107 16.264 11.397 1.00 33.83 N ATOM 408 CA THR A 67 22.286 15.540 11.845 1.00 33.70 C ATOM 409 C THR A 67 21.937 14.177 12.340 1.00 33.84 C ATOM 410 O THR A 67 22.986 13.340 12.431 1.00 34.42 O ATOM 411 CB THR A 67 22.951 16.215 13.020 1.00 33.66 C ATOM 412 OG1 THR A 67 21.981 16.451 14.046 1.00 33.90 O ATOM 413 CG2 THR A 67 23.472 17.562 12.674 1.00 33.56 C ATOM 414 N ASN A 68 20.686 13.954 12.719 1.00 34.00 N ATOM 415 CA ASN A 68 20.686 13.954 12.719 1.00 34.00 N ATOM 416 C ASN A 68 21.108 12.454 14.575 1.00 34.15 C ATOM 417 O ASN A 68 21.108 12.454 14.575 1.00 33.97 C ATOM 418 CB ASN A 68 21.281 11.330 15.008 1.00 33.83 O ATOM 418 CB ASN A 68 20.653 11.531 12.375 1.00 34.26 C ATOM 420 OD1 ASN A 68 18.512 11.104 11.239 1.00 35.12 C ATOM 420 OD1 ASN A 68 18.512 11.104 11.239 1.00 35.12 C ATOM 420 CD1 ASN A 68 20.168 11.649 10.033 1.00 36.88 N ATOM 420 CD1 ASN A 68 22.588 13.531 15.162 1.00 34.15 C ATOM 420 CD1 ASN A 68 22.588 13.531 15.162 1.00 34.16 C ATOM 420 CD LEU A 69 22.446 13.419 16.334 1.00 34.16 C ATOM 420 CD LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 420 CD LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 420 CD LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 420 CD LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 420 CD LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 420 CD LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 420 CD LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 420 CD LEU A 69 22.558 11.731 18.039 1.00 34.16 C ATOM 420 CD LEU A 69 22.558 11.731 18.039 1.00 34.16 C ATOM 420 CD LEU A 69 22.558 11.731 18.039 1.00 34.16 C ATOM 420 CD LEU A 69 22.558 11.731 18.039 1.00 34.16 C ATOM 420 CD LEU A 69 22.558 11.737 18.039 1.00 34.16 C ATOM 420 CD LEU A 69 22.558 11.730 17.854 1.00 34.16 C ATOM 423 CA LEU A 69 22.558 11.730 17.854 1.00 34.16 C ATOM 423 CA LEU A 69 22.555 12.783 17.732 1.00 34.16 C ATOM 433 CA VAL A 70 19.877 12.023 18.777 1.00 34.46 C ATOM 433 C	ATOM	403	CB	ASP A	66	19.339	16.653	8.192	1.00 33.55	С
ATOM 406 OD2 ASP A 66 20.583 17.456 6.284 1.00 35.31 O ATOM 407 N THR A 67 21.107 16.264 11.397 1.00 33.83 N ATOM 408 CA THR A 67 22.286 15.540 11.845 1.00 33.70 C ATOM 409 C THR A 67 22.808 13.340 1.00 33.84 C ATOM 410 O THR A 67 22.808 13.340 12.431 1.00 34.42 O ATOM 411 CB THR A 67 22.951 16.215 13.020 1.00 33.66 C ATOM 412 OG1 THR A 67 21.981 16.451 14.046 1.00 33.90 O ATOM 413 CG2 THR A 67 23.472 17.562 12.674 1.00 33.56 C ATOM 414 N ASN A 68 20.686 13.954 12.719 1.00 34.00 N ATOM 415 CA ASN A 68 20.320 12.676 13.312 1.00 34.15 C ATOM 416 C ASN A 68 21.108 12.454 14.575 1.00 33.97 C ATOM 417 O ASN A 68 21.281 11.330 15.008 1.00 33.83 O ATOM 418 CB ASN A 68 20.653 11.531 12.375 1.00 34.26 C ATOM 419 CG ASN A 68 19.685 11.411 11.239 1.00 34.26 C ATOM 420 OD1 ASN A 68 19.685 11.411 11.239 1.00 35.12 C ATOM 421 ND2 ASN A 68 21.598 13.531 15.162 1.00 34.15 N ATOM 422 N LEU A 69 21.598 13.531 15.162 1.00 34.15 N ATOM 423 CA LEU A 69 22.446 13.419 16.334 1.00 34.19 C ATOM 426 CB LEU A 69 22.538 11.531 12.375 1.00 34.10 C ATOM 427 CG LEU A 69 22.538 11.531 12.375 1.00 34.16 C ATOM 428 CD1 LEU A 69 22.538 11.531 18.581 1.00 34.19 C ATOM 428 CD LEU A 69 22.538 11.531 18.581 1.00 34.19 C ATOM 429 CD2 LEU A 69 22.538 11.737 18.039 1.00 34.10 C ATOM 427 CG LEU A 69 22.538 11.737 18.039 1.00 34.10 C ATOM 428 CD1 LEU A 69 23.883 16.183 18.582 1.00 34.10 C ATOM 429 CD2 LEU A 69 23.883 16.183 18.582 1.00 34.10 C ATOM 429 CD2 LEU A 69 23.883 16.183 18.582 1.00 34.10 C ATOM 429 CD2 LEU A 69 23.883 16.183 18.582 1.00 34.46 C ATOM 430 N VAL A 70 19.877 12.023 18.777 1.00 34.46 C ATOM 431 CA VAL A 70 19.877 12.023 18.777 1.00 34.46 C ATOM 432 C VAL A 70 19.870 11.223 18.865 1.00 34.46 C ATOM 433 CG VAL A 70 19.540 12.899 20.003 1.00 34.61 C ATOM 435 CG1 VAL A 70 19.540 12.899 20.003 1.00 34.61 C ATOM 435 CG1 VAL A 70 19.540 12.899 20.003 1.00 34.61 C	MOTA	404	ÇG	ASP A	66	20.397	17.484	7.508	1.00 34.00	С
ATOM 407 N THR A 67 21.107 16.264 11.397 1.00 33.83 N ATOM 408 CA THR A 67 22.286 15.540 11.845 1.00 33.70 C ATOM 409 C THR A 67 21.937 14.177 12.340 1.00 33.84 C ATOM 410 O THR A 67 22.808 13.340 12.431 1.00 34.42 O ATOM 411 CB THR A 67 22.951 16.215 13.020 1.00 33.66 C ATOM 412 OGI THR A 67 22.951 16.215 13.020 1.00 33.66 C ATOM 413 CG2 THR A 67 23.472 17.562 12.674 1.00 33.56 C ATOM 414 N ASN A 68 20.686 13.954 12.719 1.00 34.00 N ATOM 415 CA ASN A 68 20.320 12.676 13.312 1.00 34.15 C ATOM 416 C ASN A 68 21.108 12.454 14.575 1.00 33.97 C ATOM 417 O ASN A 68 21.281 11.330 15.008 1.00 33.83 O ATOM 418 CB ASN A 68 20.653 11.531 12.375 1.00 34.26 C ATOM 419 CG ASN A 68 19.685 11.411 11.239 1.00 34.26 C ATOM 420 OD1 ASN A 68 18.512 11.104 11.434 1.00 35.89 O ATOM 421 ND2 ASN A 68 18.512 11.104 11.434 1.00 35.89 O ATOM 422 N LEU A 69 21.598 13.531 15.162 1.00 34.15 C ATOM 423 CA LEU A 69 21.598 13.531 15.162 1.00 34.16 C ATOM 426 CB LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 426 CB LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 427 CG LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 428 CD1 LEU A 69 23.652 14.795 18.125 1.00 34.16 C ATOM 429 CD2 LEU A 69 23.883 16.183 16.581 1.00 34.15 N ATOM 428 CD1 LEU A 69 23.883 16.183 17.732 1.00 34.66 C ATOM 430 N VAL A 70 19.877 12.023 18.777 1.00 34.46 C ATOM 431 CA VAL A 70 19.877 12.023 18.777 1.00 34.46 C ATOM 432 CVAL A 70 19.877 12.023 18.777 1.00 34.46 C ATOM 433 C VAL A 70 19.877 12.023 18.777 1.00 34.46 C ATOM 434 CB VAL A 70 19.877 12.023 18.700 34.61 C ATOM 433 C CVAL A 70 19.877 12.023 18.705 1.00 34.66 C ATOM 434 CB VAL A 70 19.877 12.023 18.705 1.00 34.66 C ATOM 435 CGI VAL A 70 19.540 12.899 20.003 1.00 34.61 C ATOM 435 CGI VAL A 70 19.540 12.899 20.003 1.00 34.61 C ATOM 435 CGI VAL A 70 19.540 12.899 20.003 1.00 34.61 C ATOM 435 CGI VAL A 70 18.654 11.370 13.939 19.706 1.00 34.21 C	MOTA	405	OD1	ASP A	66	21.124	18.232	8.188	1.00 35.03	0
ATOM 407 N THR A 67 21.107 16.264 11.397 1.00 33.83 N ATOM 408 CA THR A 67 22.286 15.540 11.845 1.00 33.70 C ATOM 409 C THR A 67 21.937 14.177 12.340 1.00 33.84 C ATOM 410 O THR A 67 22.808 13.340 12.431 1.00 34.42 O ATOM 411 CB THR A 67 22.951 16.215 13.020 1.00 33.66 C ATOM 412 OGI THR A 67 22.951 16.215 13.020 1.00 33.66 C ATOM 413 CG2 THR A 67 23.472 17.562 12.674 1.00 33.56 C ATOM 414 N ASN A 68 20.686 13.954 12.719 1.00 34.00 N ATOM 415 CA ASN A 68 20.320 12.676 13.312 1.00 34.15 C ATOM 416 C ASN A 68 21.108 12.454 14.575 1.00 33.97 C ATOM 417 O ASN A 68 21.281 11.330 15.008 1.00 33.83 O ATOM 418 CB ASN A 68 20.653 11.531 12.375 1.00 34.26 C ATOM 419 CG ASN A 68 19.685 11.411 11.239 1.00 34.26 C ATOM 420 OD1 ASN A 68 18.512 11.104 11.434 1.00 35.89 O ATOM 421 ND2 ASN A 68 18.512 11.104 11.434 1.00 35.89 O ATOM 422 N LEU A 69 21.598 13.531 15.162 1.00 34.15 C ATOM 423 CA LEU A 69 21.598 13.531 15.162 1.00 34.16 C ATOM 426 CB LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 426 CB LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 427 CG LEU A 69 22.538 11.737 18.039 1.00 34.16 C ATOM 428 CD1 LEU A 69 23.652 14.795 18.125 1.00 34.16 C ATOM 429 CD2 LEU A 69 23.883 16.183 16.581 1.00 34.15 N ATOM 428 CD1 LEU A 69 23.883 16.183 17.732 1.00 34.66 C ATOM 430 N VAL A 70 19.877 12.023 18.777 1.00 34.46 C ATOM 431 CA VAL A 70 19.877 12.023 18.777 1.00 34.46 C ATOM 432 CVAL A 70 19.877 12.023 18.777 1.00 34.46 C ATOM 433 C VAL A 70 19.877 12.023 18.777 1.00 34.46 C ATOM 434 CB VAL A 70 19.877 12.023 18.700 34.61 C ATOM 433 C CVAL A 70 19.877 12.023 18.705 1.00 34.66 C ATOM 434 CB VAL A 70 19.877 12.023 18.705 1.00 34.66 C ATOM 435 CGI VAL A 70 19.540 12.899 20.003 1.00 34.61 C ATOM 435 CGI VAL A 70 19.540 12.899 20.003 1.00 34.61 C ATOM 435 CGI VAL A 70 19.540 12.899 20.003 1.00 34.61 C ATOM 435 CGI VAL A 70 18.654 11.370 13.939 19.706 1.00 34.21 C	MOTA	406	OD2	ASP F	4 66	20.583	17.456	6.284	1.00 35.31	0
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ATOM 436 CG2 VAL A 70 18.493 13.939 19.706 1.00 34.21 C										С
ATOM 437 N TYR A 71 18.833 10.762 17.033 1.00 34.98 N										
	MOTA	437	N	TYR	A 71	18.833	10.762	17.033	1.00 34.98	N

									•		
ATOM	438	CA	TYR	Α	71	17.779	10.041	16.352	1.00 35.19		С
MOTA	439	С	TYR	A	71	17.051	9.086	17.305	1.00 35.24		Č
MOTA	440	0	TYR	A	71	15.837	9.148	17.421	1.00 35.61		0
MOTA	441	CB	TYR	A	71	18.337	9.291	15.137	1.00 35.26	4	С
MOTA	442	CG	TYR	Α	71	17.352	8.278	14.618	1.00 35.95		С
ATOM	443	CD1			71	16.155	8.696	14.055	1.00 35.96		C
MOTA	444	CD2	TYR	A	71	17.584	6.915	14.731	1.00 34.66		Ċ
ATOM	445	CE1	TYR	Α	71	15.239		13.610	1.00 35.86		Č
MOTA	446	CE2	TYR	Α	71	16.664 [°]	6.011	14.281	1.00 34.47		Č
MOTA	447	CZ	TYR	A	71	15.485	6.463	13.724			Č
MOTA	448	OH	TYR	Α	71	14.518	5.589	13.248	1.00 38.92		ō
MOTA	449	N	PRO	Α	72	17.774	8.211	17.993	1.00 35.15		N
ATOM	450	CA	PRO	Α	72	17.141	7.271	18.924	1.00 35.16		C
ATOM		С	PRO	A·	72	16.357	7.923	20.068	1.00 35.14		Ċ
MOTA	452	0	PRO	Α	72	15.473	7.294	20.643	1.00 34.97		ō
MOTA	453	CB	PRO	Α	72	18.327	6.475	19.487	1.00 35.18		Č
MOTA	454	CG	PRO	Α	72 .	19.433	6.677	18.524	1.00 35.26		Ċ
ATOM	455	CD	PRO	A	72	19.233	8.031	17.938	1.00 35.29		Č
ATOM	456	N	ALA	A	73	16.657	9.169	20.401	1.00 35.18		N
ATOM	457	CA	ALA	A	73	15.967	9.803	21.512	1.00 35.21		C
ATOM	458	С	ALA	\mathbf{A}	73	14.657	10.414	21.097	1.00 35.08		Č
ATOM		0	ALA	Α	73	13.890	10.862	21.934	1.00 34.86		ō
MOTA		CB	ALA	A	73	16.829	10.864	22.135	1.00 35.37		C
MOTA		N	LEU	Α	74	14.370	10.434	19.812	1.00 35.25		N
ATOM		CA	LEU	Α	74	13.142	11.090	19.399	1.00 35.54	•	C
MOTA		С	LEU	Α.	74 .	11.903	10.434	19.958	1.00 35.66		Ċ
ATOM		0	LEU	A	74	10.893	11.088	20.118	1.00 35.64		0
MOTA		CB	LEU	A	74 ·	13.044	11.190	17.894	1.00 35.31		. C
MOTA		CG	LEU	A	74 -	14.161	12.046	17.333	1.00 36.48		C
MOTA		CD1			74	13.887	12.277	15.890	1.00 37.76	•	C
ATOM			LEU		74	14.300	13.394	18.076	1.00 37.06		С
MOTA		N	LYS		75	11.979	9.151	20.282	1.00 36.19		N
ATOM		CA	LYS		75	10.795	8.453	20.767	1.00 36.36		С
ATOM		С	LYS		75	10.566	8.710	22.246	1.00 36.85		С
ATOM		0	LYS		75	9.491	8.437	22.765	1.00 37.12		0
ATOM		CB	LYS		75	10.904	6.956	20.505	1.00 36.04		С
ATOM		CG	LYS		75	12.060	6.284	21.216	1.00 35.77		С
ATOM		CD	LYS		75	12.245	4.829	20.782	1.00 34.46		С
ATOM			LYS		75	13.720	4.460	20.710	1.00 33.42		С
ATOM		NZ	LYS		75	14.375	4.536	22.036	1.00 32.34		N
ATOM		N	TRP	A	76	11.578	9.244	22.920	1.00 37.24		N
ATOM		CA	TRP		76	11.481	9.510	24.345	1.00 37.30	·	С
MOTA		C	TRP		76	10.274	10.369	24.700	1.00 37.42	•	Ċ
ATOM		0	TRP		76	9.917	11.306	23.984	1.00 37.54		0
ATOM		CB	TRP		76	12.728	10.247	24.838	1.00 37.12		С
ATOM		CG	TRP		76	13.980	9.446		1.00 36.77		С
ATOM			TRP		76	14.142	8.176	24.359	1.00 37.03		С
ATOM			TRP		76	15.255	9.864	25.291	1.00 36.31		Ç
MOTA			TRP		76	15.445	7.776	24.527	1.00 36.52		N
ATOM			TRP		76	16.147	8.801	25.097	1.00 36.08		С
ATOM			TRP		76	15.737	11.040	25.864	1.00 36.23		C
ATOM			TRP		76	17.480	8.881	25.443	1.00 36.27		С
ATOM			TRP		76	17.055	11.113	26.209	1.00 36.35		C
ATOM			TRP		76	17.915	10.045	25.996	1.00 36.41		С
ATOM		N	ASP		77 ·	9.662	10.015	25.820	1.00 37.42		N
ATOM		CA	ASP		77	8.591	10.768	26.435	1.00 37.36	•	С
ATOM		C	ASP		77 ·	8.707	10.370	27.907	1.00 37.09		С
ATOM		O	ASP		77	9.628	9.647	28.260	1.00 37.04		0
ATOM		CB	ASP		77	7.245	10.377	25.834	1.00 37.48		С
ATOM ATOM		CG	ASP		77	6.990	8.888	25.903	1.00 38.01		С
MIOM	498	ODI	ASP	A	77	7.704	8.191	26.658	1.00 38.42		0

7.000	400	000	A O D	75	77	6.093	8.319	25.244	1.00	39 67		0
MOTA	499	OD2			77				1.00			N
ATOM	500		LEU .		78	7.789	10.798	28.763				Ċ
ATOM	501		LEU		78	7.913	10.496	30.182	1.00			C
ATOM	502		LEU		78	7.729	9.026	30.464	1.00			
ATOM	503		LEU		78	8.456	8.426	31.260	1.00			0
ATOM	504	CB	LEU	Ą	78 ·	6.903	11.296	30.974	1.00			С
ATOM	505	CG	LEU	Α	78	7.119	12.796	30.863	1.00	36.49		С
MOTA	506	CD1	LEU	Α	78	6.008	13.510	31.594	1.00	36.63		.C
ATOM	507	CD2			78	8.494	13.194	31.399	1.00	36.10		С
ATOM	508		GLU		79	6.748	8.433	29.815	1.00	36.81		N
ATOM	509		GLU		79	6.505	7.030	30.041	1.00	36.97		С
ATOM	510		GĽU		79	7.737	6.176	29.738		36.75		C
	511		GLU		79	8.151	5.373	30.572		36.84		Ö
ATOM						5.323	6.560	29.214		37.25		č
MOTA	512		GLU		79							c
MOTA	513		GLU		79	4.937	5.137	29.540		37.93		C
ATOM	514		GLU		79	3.729	4.681	28.768		38.61		
MOTA	515		GLU		79	3.381	5.352	27.775		38.32	•	0
MOTA	516	OE2	GLU	Α	79	3.131	3.654	29.166		40.10		0
MOTA	517	N	TYR	Α	80	8.318	6.337	28.553		36.50	,	N
MOTA	518	CA	TYR	Α	80	9.489	5.549	28.176	1.00	36.32		С
ATOM	519	С	TYR	Α	80	10.644	5.804	29.123	1.00	36.27		С
MOTA	520	Ó	TYR		80	11.343	4.872	29.516	1.00	36.15		0
ATOM	521	CB	TYR		80	9.921	5.889	26.751		36.39		С
ATOM	522	CG	TYR		80	11.180	5.202	26.228		36.06		C
MOTA	523	CD1			80	11.100	4.000	25.557		36.22		C
						12.432	5.793	26.349		35.91		Č
ATOM	524	CD2	TYR		80			25.051		36.52		Ċ
MOTA	525	CE1			80	12.225	3.380					C
ATOM	526		TYŖ		80	13.568	5.179	25.844		36.04		c
MOTA	527	CZ	TYR		80	13.454	3.967	25.190		36.46		
ATOM	528	OH	TYR		80	14.561	3.321	24.673		35.81		0
MOTA	529	N	LEU	Α	,81	10.846	7.064	29.493		36.13		N
ATOM	530	CA	LEU	A	81	11.971	7.408	30.353		36.22		C
MOTA	531	С	LEU	Α	81	11.777	6.827	31.747	1.00	36.13		С
MOTA	532	0	LEU	Α	81	12.706	6.259	32.325	1.00	35.90		0
MOTA	533	CB	LEU	·A	81	12.208	8.930	30.406	1.00	36.22		C
MOTA	534	CG	LEU	Α	81	12.774	9.568	29.121	1.00	36.35	•	C
MOTA	535		LEU		81	12.880		29.274	1.00	36.49		С
ATOM	536		LEU		81	14.132		28.718		36.18		С
ATOM	537	N	GLN		82	10.569		32.280		36.15	•	N
ATOM	538	CA	GLN		82	10.284		33.597		36.29		C
	539	C	GLN		82	10.575		33.605		36.25		C
MOTA								34.515				.0
ATOM	540	0	GLN			11.210						Č
ATOM	541	CB	GLN			8.838				36.38		c
MOTA	542	CG	GLN			8.418				37:00	••	
ATOM	543	CD	GL			7.191				37.85		C
MOTA	544		. GLN			6.640				38.24		0
MOTA	545	NE2	GL1			6.754				38.93		N
MOTA	546	N	GL	JA	83	10.136				36.46		N
MOTA	547	CA	GL	JA	83	10.366	2.807			36.59		С
ATOM	548	С	GL	JA	83	11.843	3 2.424	32.307	1.00	36.50		С
ATOM .	549			A C		12.228			1.00	36.55		0
MOTA	550		GL			9.568				36.57		С
ATOM	551			U A		9.49				36.95		С
ATOM	552			U A		8.73				37.61		C
	553		L GL			7.92				37.88		Ö
MOTA						8.93				37.54		ő
ATOM	554		2 GL									N
ATOM	555			N A		. 12.680				36.58		C
ATOM	556			N A		14.04				36.62		
ATOM	557			N A		15.21				36.66		C
MOTA	558				84	16.34				36.62		0
MOTA	559	CB	AS	N A	84	14.21	1 2.936	29.960	1.00	36.62	•	С

ATOM	560	CG	ASN	A	84	13.362	1:902	29.286	1.00 36.37	С
MOTA	561		ASN		84	13.352	0.733	29.683	1.00 36.46	0
ATOM	562		ASN		84	12.644	2.317	28.247	1.00 35.65	N
MOTA	563	N	ILE		85	14.975	4.920	32.557	1.00 36.80	N
ATOM	564	CA	ILE		85	16.125	5.730	32.885	1.00 37.13	С
ATOM	565	C	ILE		85	16.834	5.365	34.180	1.00 37.28	С
MOTA	566	0	ILE		85	17.793	6.022	34.568	1.00 37.74	0
ATOM	567	CB	ILE		85	15.752	7.184	32.874	1.00 37.21	С
MOTA MOTA	568				85	16.958	8.009	32.445	1.00 37.55	C
ATOM	569 570	CG2 CD1			85	15.241	7.593	34.222	1.00 37.38	C
ATOM	571	N	ILE GLY		85 86	16.623	9.467	32.195	1.00 37.68	C
ATOM	572	CA	GLY		86	16.383 17.089	4.326	34.855	1.00 37.29	N
ATOM	573	C.	GLY		86	16.553	3.892 4.496	36.038 37.308	1.00 37.39	C
ATOM	574	0	GLY		86	15.583	5.265	37.290	1.00 37.43 1.00 37.34	C 0
ATOM	575	N	ASN		87	17.212	4.167	38.414	1.00 37.34	N
ATOM	576	CA	ASN		87	16.750	4.602	39.716	1.00 37.34	C
ATOM	577	С	ASN		87	17.701	5.603	40.357	1.00 37.39	C
MOTA	578	0	ASN		87	17.740	5.742	41.578	1.00 37.39	Ō
ATOM	579	СВ	ASN		87	16.545	3.399	40.612	1.00 37.40	Č
MOTA	580	N	GLY	Α	.88	18.451	6.321	39.529	1.00 37.47	И
MOTA	581	CA	GLY	Α	88	19.405	7.296	40.028	1.00 37.41	C
MOTA	582	С	GLY	Α	88	18.686	8.554	40.450	1.00 37.30	C
MOTA	583	0	GLY	Α	88	17.500	8.709	40.171	1.00 37.36	0
MOTA	584	N	ASP		89	19.390	9.453	41.125	1.00 37.26	N
MOTA	585	CA	ASP		89	18.780	10.716	41.531	1.00 37.21	С
MOTA	586	C	ASP		89	18.726	11.681	40.355	1.00 36.91	C
MOTA	587	0	ASP		89	19.607	11.654	39.500	1.00 36.62	0
ATOM	588	CB	ASP		89	19.563	11.346	42.680	1.00 37.24	С
ATOM	589	CG	ASP		89	19.277	10.690	44.000	1.00 37.24	С
ATOM	590		ASP		89	18.398	9.802	44.044	1.00 37.14	0
ATOM ATOM	591		ASP		89	19.876	11.002	45.047	1.00 37.98	0
MOTA	592 593	N CA	PHE		90	17.667	12.492	40.295	1.00 36.88	N
ATOM	594	CA	PHE PHE		90 90	17.554	13.570	39.298	1.00 36.87	С
ATOM	595	0	PHE		90	17.327 16.455	14.926	39.942	1.00 36.79	C
ATOM	596	СВ	PHE		90	16.420	15.080 13.308	40.795 38.321	1.00 36.69	0
ATOM	597	CG	PHE		90	16.712	12.210	37.371	1.00 36.70 1.00 36.83	C
ATOM	598	CD1			90	16.551	10.901	37.757	1.00 36.83	C
MOTA	599		PHE		90	17.191	12.479	36.102	1.00 30.07	C
ATOM	600		PHE		90	16.827	9.885	36.899	1.00 37.27	Č
ATOM	601		PHE		90	17.475	11.449	35.238	1.00 36.82	Č
MOTA	602	CZ	PHE		90	17.291	10.150	35.642	1.00 36.06	C
MOTA	603	N	SER	Α	91	18.123	15.905	39.529	1.00 36.92	N
MOTA	604	CA	SER	A	91	17.971	17.266	40.027	1.00 36.99	C
ATOM	605	С	SER	A	91	16.738	17.923	39.428	1.00 37.10	С
MOTA	606	0	SER		91	16.586	17.985	38.206	1.00 36.78	0
MOTA	607	CB	SER		91	19.200	18.105	39.699	1.00 36.86	C
MOTA	608	OG	SER		91 '	20.350	17.616	40.358	1.00 36.54	0
ATOM	609	N	VAL		92	15.857	18.402	40.303	1.00 37.42	N
ATOM	610	CA	VAL		92	14.660	19.106	39.876	1.00 37.75	C
ATOM	611	C	VAL		92	14.509	20.468	40.545	1.00 38.10	С
MOTA	612	O	VAL		92	14.472	20.589	41.768	1.00 38.08	0
MOTA	613	CB	VAL		92	13.406	18.303	40.159	1.00 37.63	C
MOTA MOTA	614 615		VAL		92	12.197	19.034	39.621	1.00 37.42	. с
ATOM	615 616		VAL		92	13.515	16.946	39.527	1.00 37.78	C
ATOM	617	N CA	TYR		93	14.384	21.487	39.709	1.00 38.59	. N
ATOM	618	CA	TYR TYR		93 93	14.220 12.784	22.849	40.166	1.00 38.91	C
ATOM	619	0	TYR		93	12.784	23.173 22.786	40.219 39.343	1.00 39.41	C
ATOM	620	СВ	TYR		93	14.883	23.799	39.343	1.00 39.64	0
	720	JD	T T T/	4-3	23	14.003	23.133	33.202	1.00 38.84	С

ATOM	621	CG	TYR A	A	93	16.332	23.588	39.288	1.00 3	8.25		С
ATOM			TYR A		93	17.044	24.122	40.334	1.00 3	8.21		С
ATOM	623	CD2	TYR A	A	93	16.968	22.750	38.415	1.00 3	7.50		С
MOTA	624	CE1	TYR A	A	93	18.362	23.893	40:464	1.00 3			С
MOTA	625		TYR A		93	18.287	22.512	38.534	1.00 3			С
MOTA	626		TYR I		93	18.987	23.090	39.557	1.00 3			C
MOTA	627		TYR Z	•	93	20.322	22.836	39.677	1.00 3			0
MOTA	628	N	SER		94	12.422	23.935	41.228	1.00 4			N
MOTA	629	CA	SER .		94	11.043	24.274	41.416	1.00 4			C
MOTA	630	C	SER :		94	11.020	25.773	41.426	1.00 4			С
ATOM	631	0	SER .		94	11.962	26.384	41.896 42.730	1.00 4			0 C
ATOM	632	CB	SER .		94	10.539	23.693 23.874	42.730	1.00 4			Ö
MOTA	633	OG	SER .		94 95	9.139 9.974	26.374	42.838	1.00 4			N
MOTA MOTA	634 635	N CA	ALA ALA		95	9.899	27.824	40.856	1.00 4		•	c
ATOM	636	C	ALA		95 ·	8.483	28.343	40.826	1.00 4			č
ATOM	637	ō	ALA		95	7.573	27.699	40.309	1.00 4			٠0
ATOM	638	CB	ALA		95	10.630	28.350	39.668	1.00 4		•	С
ATOM	639	N	SER		96	8.328	29.549	41.350	1.00 4			N
MOTA	640	CA	SER		96	7.034	30.200	41.413	1.00 4	11.05		С
ATOM	641	С	SER	A	96	6.834	31.208	40.305	1.00 4	10.72		С
ATOM .	642	0	SER	A	96	5.833	31.912	40.277	1.00 4			0
ATOM	643	CB	SER	Α	96	6.902	30.938	42.731	1.00			С
MOTA	644	OG	SER		96	5.767	31.779	42.693	1.00		•	0
MOTA	645	N	THR		97	7.808	31.314	39.423	1.00			N
MOTA	646	CA	THR		97	7.710	32.209	38.292	1.00			C
MOTA	647	С	THR		97	8.073	31.368	37.113	1.00			C 0
ATOM	648	0	THR		97	8.582	30.274	37.279 38.393	1.00			C
MOTA	649	CB	THR		97 97	8.732 8.905	33.336 33.946	37.105	1.00			Ö
MOTA	650 651	OG1 CG2			97 97	10.145	32.779	38.718	1.00			Č
ATOM ATOM	652	N CGZ	HIS		98	7.862	31.874	35.915	1.00			N
ATOM	653	CA	HIS		98	8.257	31.112	34.754	1.00			Ċ
ATOM	654	C	HIS		98	9.765	31.163	34.543		39.41 [°]		С
MOTA	655	Ō	HIS		98	10.299	30.423		1.00			0
ATOM	656	СВ	HIS		98	7.576	31.646	33.516	1.00	38.95		С
MOTA	657	CG	HIS		98	7.807	33.104	33.290	1.00			C
MOTA	658	ND1	HIS	Α	98	7.095	34.081	33.950		37.36		N
MOTA	659	CD2	HIS	A	98	8.672	33.753	32.477		38.57		С
MOTA	660		. HIS		98	7.509	35.268	33.550		37.33		· C
MOTA	661		HIS		98	8.463	35.098	32.654		37.37		N
ATOM	662	N	LYS		99	10.452	32.021	35.294		39.52		N
ATOM	663	CA	LYS		99	11.881	32.184	35.105		39.98		C
MOTA	664	C	LYS		99	12.749	31.364 31.554	36.029 37.246		40.38		Ö
ATOM ATOM	665 666	O	LYS LYS		99 99	12.744 12.281	33.631	35.297		40.10		c
MOTA	667	CB CG	LYS		99	11.814		34.219		40.15	•	Č
ATOM	668	CD	LYS		99.	12.537	35.820	34.337		40.36		Ċ
ATOM	669	CE	LYS		99	11.725		35.072		41.10		C
ATOM	670	NZ	LYS		99	10.975				41.52		N
ATOM	671	N			100	13.541				40.77		N
ATOM	672				100	14.450				41.12		С
ATOM	673				100	15.893	30.159	36.218		41.78		С
MOTA	674				100	16.808				42.13		0
MOTA	675				100	14.418				40.86		C
MOTA	676				100	13.211				40.53		C
MOTA	677		1 PHE			12.040				39.76		C
MOTA	678		2 PHE			13.249				39.54		C
MOTA	679		1 PHE			10.942				39.56 39.79		C
MOTA	680		2 PHI			12.155 10.995				39.79		C
ATOM	681	CZ	PHI	ı A	100	10.333	20.004	50.002	. 1.00	JJ.J.		C

ATOM	682	N	LEU A	A 10	oi	16.1	L24	31.34	17	36.7	47	1.00	42.2	23		N
ATOM	683	CA	LEU A	A 10	01	17.5	501	31.80	00	36.8		1.00	42.7	4		С
ATOM	684	С	LEU A	A 10	01	18.4		30.78		37.5		1.00	43.2	27		С
MOTA	685	0	LEU Z	A 10	01 .	18.2		30.39		38.7		1.00				0
ATOM	686	CB	LEU Z	A 10	01	17.5	549	33.09	97	37.6		1.00	42.9	90		С
ATOM	687		LEU 2			18.9		33.80		37.7		1.00		_		C
ATOM	688		LEU 2			19.		34.2		36.4		1.00				C
MOTA	689		LEU			18.		34.9		38.7		1.00				Č
ATOM	690	N	TYR			19.		30.3		36.8		1.00				N
ATOM	691	CA	TYR			20.		29.5		37.3		1.00				C
ATOM .	692	C	TYR			21.		30.1		38.4		1.00				Č
ATOM	693	o	TYR .			21.		31.3		38.3		1.00				ŏ
ATOM	694	СВ	TYR			21.		29.2		36.1		1.00				c
ATOM	695	CG	TYR			22.		28.4		36.7		1.00				c
ATOM	696	CD1	TYR			22.		27.0		37.0		1.00				č
ATOM	697	CD2	TYR			23.		29.0		36.9		1.00				č
ATOM	698	CE1	TYR			23.		26.3		37.5		1.00				c
ATOM	699	CE2	TYR			24		28.3		37.4		1.00				č
ATOM	700	CZ	TYR			24.		26.9		37.7		1.00				č
ATOM	701	ОН	TYR			25.		26.3		38.2		1.00				ŏ
ATOM	702	N	TYR			21.		29.4		39.5		1.00				N
MOTA	703	CA	TYR			22.		29.9		40.5		1.00				C
ATOM	704	C	TYR				561	28.8		41.1		1.00				c
ATOM	705	Ö	TYR				165	27.7		41.3		1.00				0
ATOM	706	CB	TYR				922	30.6		41.6		1.00				C
ATOM	707	CG	TYR			20.		29.6		42.2		1.00				C
ATOM	708	CD1					770	29.4		41.6		1.00				C
ATOM	709	CD2					306	28.9		43.3		1.00				C
ATOM	710		TYR				880	28.5		42.		1.00				C
ATOM	711		TYR				426	28.0		43.9		1.00				C
ATOM	712	CZ	TYR													c
ATOM	713	OH					203	27.8		43.2			48.			
ATOM	713	N	TYR ASP				287	26.9		43.			51.			0
ATOM	715	CA	ASP				786	29.3 28.3		41.			41.			N
ATOM	716		ASP				829			41.			40.			C
ATOM	717	o ·	ASP				924 430	28.3		43.			40.			0
ATOM	718	СВ	ASP				110	28.9					40.		•	
. ATOM	719	CG	ASP				306	28.1		41.						C
ATOM	720		ASP				270	27.4					41.			0
ATOM	721		ASP				337	28.0		42. 40.			42.			0
ATOM	722	N	GLU				446	27.2		43.			40.			Ŋ
ATOM	723	CA	GLU				368									_
ATOM	724	C	GLU				734	27.0		45. 45.			40. 39.			C
ATOM	725	Ö	GLU				803	27.7		47.			39.			0
ATOM .	726	СВ	GLU				769	25.6		45.			40.			
ATOM	727	CG	GLU				247	25.5		45.			40.			C C
ATOM	728	CD	GLU				708	24.1		45.						C
ATOM	729		GLU				. 138	23.2			986) 42.) 43:			0
ATOM	730		GLU				.842	23.9			322		42.			0
ATOM	731	N	LYS				.824	26.8			204		39.			
ATOM	732	CA	LYS								831					N C
ATOM	733	CA	LYS				.141 .427	27.0 28.4			190		39. 39.			C
ATOM	734	0														
MOTA	735		LYS				.165	28.			128		39.			0
		CB	LYS				.302	26.5			945		39.			C
ATOM	736	CG	LYS				.444	25.0			731		39.			C
MOTA	737	N	LYS				.856	29.3			438		39.			N
ATOM ATOM	738 739	CA	LYS				.140	30.			663		39.			C
		C	LYS				.151	31.4			607		40.			C
ATOM ATOM	740 741	O	LYS				.279	32.0			883		40.			0
ATOM	741	CB	LYS				.161	31.5			325		39.			C
ATOM	142	CG	LYS	Α.	101	30	.390	31.	エココ	43.	455	1.00	38.	46		С

ATOM	743 CD LYS A 107	30.299 31.737 42.029 1.00 36.98
ATOM	744 CE LYS A 107	31.643 31.632 41.292 1.00 36.36
MOTA	745 NZ LYS A 107	31.553 31.935 39.819 1.00 35.12
ATOM	746 N MET A 108	27.197 30.697 47.148 1.00 40.92
ATOM	747 CA MET A 108	26.165 31.316 47.978 1.00 41.42
ATOM	748 C MET A 108	26.675 31.937 49.258 1.00 42.03
	749 O MET A 108	26.142 32.952 49.704 1.00 42.33
ATOM		25.006 30.366 48.210 1.00 41.31
ATOM		24.285 30.179 46.892 1.00 41.95
ATOM	751 CG MET A 108	- - · - · -
ATOM	752 SD MET A 108	
MOTA	753 CE MET A 108	
MOTA	754 N ALA A 109	27.737 31.382 49.816 1.00 42.84
MOTA	755 CA ALA A 109	28.282 31.912 51.064 1.00 43.65
MOTA	756 C ALA A 109	28.655 33.387 50.963 1.00 44.40
MOTA	757 O ALA A 109	28.321 34.195 51.823 1.00 44.44
MOTA	758 CB ALA A 109	29.486 31.107 51.476 1.00 43.66
MOTA	759 N ASN A 110	29.332 33.729 49.882 1.00 45.46
ATOM	760 CA ASN A 110	29.817 35.084 49.665 1.00 46.25
MOTA	761 C ASN A 110	28.789 36.154 49.317 1.00 46.26
ATOM	762 O ASN A 110	29.163 37.304 49.066 1.00 46.51
ATOM	763 CB ASN A 110	30.841 35.036 48.543 1.00 46.62
ATOM	764 CG ASN A 110	32.024 34.145 48.886 1.00 47.94
MOTA	765 OD1 ASN A 110	32.474 34.093 50.045 1.00 48.12
ATOM	766 ND2 ASN A. 110	32.530 33.432 47.883 1.00 48.75
ATOM	767 N PHE A 111	27.517 35.786 49.228 1.00 46.12
ATOM	768 CA PHE A 111	26.470 36.795 49.057 1.00 45.97
MOTA	769 C PHE A 111	25.267 36.385 49.889 1.00 46.17
ATOM	770 O PHE A 111	24.217 36.002 49.361 1.00 46.25
	771 CB PHE A 111	26.072 36.978 47.599 1.00 45.55
ATOM		27.076 37.718 46.777 1.00 44.32
ATOM		28.269 37.123 46.419 1.00 43.65
ATOM	773 CD1 PHE A 111	
ATOM	774 CD2 PHÉ A 111	
MOTA	775 CE1 PHE A 111	
MOTA	776 CE2 PHE A 111	-
ATOM	777 CZ PHE A 111	28.911 39.068 45.177 1.00 43.00
MOTA	778 N GLN A 112	25.434 36.479 51.200 1.00 46.35
MOTA	779 CA GLN A 112	24.401 36.052 52.130 1.00 46.52
MOTA	780 C GLN A 112	23.040 36.638 51.754 1.00 46.68
ATOM	781 O GLN A 112	22.019 35.995 51.968 1.00 46.87
MOTA	782 CB GLN A 112	24.774 36.438 53.567 1.00 46.62
MOTA	783 CG GLN A 112	
MOTA	784 CD GLN A 112	26.418 34.554 54.125 1.00 48.05
MOTA	785 OE1 GLN A 112	25.834 33.762 53.372 1.00 47.89
MOTA	786 NE2 GLN A 112	27.271 34.158 55.075 1.00 48.55
MOTA	787 N ASN A 113	23.019 37.836 51.168 1.00 46,80
ATOM	788 CA ASN A 113	21.750 38.463 50.793 1.00 46.89
MOTA	789 C ASN A 113	21.104 37.951 49.517 1.00 47.08
MOTA	790 O ASN A 113.	20.105 38.521 49.077 1.00 47.55
MOTA	791 CB ASN A 113	21.898 39.976 50.682 1.00 46.69
ATOM	792 CG ASN A 113	22.258 40.604 52.001 1.00 46.91
ATOM	793 OD1 ASN A 113	22.085 39.982 53.055 1.00 46.08
ATOM	794 ND2 ASN A 113	22.767 41.837 51.962 1.00 46.59
MOTA	795 N PHE A 114	21.651 36.908 48.903 1.00 47.08
ATOM	796 CA PHE A 114	21.012 36.379 47.706 1.00 47.01
MOTA	797 C PHE A 114	19.986 35.364 48.145 1.00 47.11
ATOM	798 O PHE A 114	20.293 34.449 48.916 1.00 47.34
ATOM	799 CB PHE A 114	21.995 35.713 46.764 1.00 46.83
ATOM	800 CG PHE A 114	21.342 35.132 45.555 1.00 47.03
	801 CD1 PHE A 114	20.674 35.953 44.655 1.00 47.22
MOTA	802 CD2 PHE A 114	21.376 33.761 45.318 1.00 47.97
ATOM	803 CE1 PHE A 114	20.060 35.422 43.522 1.00 47.53
MOTA	OOD CET ENE WILL	20,000 00,122 10,022 2,0000

ATOM	804	CE2	PHE A	A	114	20.763	33.212	44.177	1.00 47.83	С
ATOM	805		PHE A			20.104	34.044	43.282	1.00 47.67	Č
ATOM	806		LYS A			18.763	35.530	47.662	1.00 46.94	Й
MOTA	807		LYS 2			17.683	34.628	48.029	1.00 46.64	C C
ATOM	808		LYS 2			17.109	34.063	46.744	1.00 46.38	Ċ
MOTA	809		LYS			16.351	34.744	46.046	1.00 46.75	ő
MOTA	810		LYS			16.613	35.372	48.835	1.00 46.60	c
MOTA	811	N	PRO .			17.445	32.813	46.449	1.00 45.84	N
ATOM	812	CA	PRO .			17.079	32.192	45.165	1.00 45.70	C
ATOM	813	С	PRO .			15.576	32.139	44.937	1.00 45.44	Č
ATOM	814	0	PRO .			14.827	31.956	45.892	1.00 45.46	Ö
ATOM	815	СВ	PRO .			17.640	30.761	45.260	1.00 45.71	Č
ATOM	816	CG	PRO .			18.435	30.689	46.536	1.00 45.66	Č
ATOM	817	CD	PRO			18.137	31.890	47.359	1.00 45.75	, c
ATOM	818	N	ARG			15.154	32.307	43.688	1.00 45.73	. O
ATOM	819	CA	ARG			13.742	32.232	43.332	1.00 45.27	C
ATOM	820	C	ARG			13.291	30.791	43.104	1.00 45.10	c
ATOM	821	ŏ	ARG			12.096	30.500	43.207	1.00 45.12	o
ATOM	822	СВ	ARG			13.467	33.059	42.097	1.00 45.46	c
ATOM	823	N	SER			14.238	29.902	42.796	1.00 43.20	N
ATOM	824	CA	SER			13.944	28.480	42.790	1.00 44.78	C
ATOM	825	C	SER			14.782	27.583	43.509	1.00 44.60	C
ATOM	826	Ö	SER			15.925	27.921	43.816	1.00 44.83	0
ATOM	827	СВ	SER			14.303	28.072	41.184	1.00 44.44	c
ATOM	828	OG	SER			15.651	27.624	41.186	1.00 44.44	0
ATOM	829	N	ASN			14.241	26.428	43.899	1.00 44.33	
ATOM	830	CA	ASN			14.969	25.472	44.728	1.00 43.72	N
MOTA	831	C	ASN			15.295	24.196	43.953	1.00 43.72	C
ATOM	832	Ö	ASN			14.576	23.821	43.933		
ATOM	833	СВ	ASN			14.147	25.078	45.955	1.00 43.23 1.00 44.03	O C
ATOM	834	CG	ASN			13.514	26.264	46.646	1.00 44.80	C
ATOM	835		ASN			14.207	27.129	47.197	1.00 44.80	
ATOM	836		ASN			12.184	26.303	46.640		0
ATOM	837	N	ARG			16.380	23.533	44.337	1.00 45.18 1.00 42.37	N
ATOM	838	CA	ARG			16.778	22.278	43.716	1.00 42.37	. N C
ATOM	839	C	ARG			16.368	21.162	44.656	1.00 41.09	C
ATOM	840	Õ	ARG			16.577	21.267	45.859	1.00 41.20	0
ATOM	841	СВ	ARG			18.299	22.239	43.504	1.00 41.40	C
ATOM	842	CG	ARG			18.827	21.002	42.754	1.00 41.70	. 0
ATOM	843	CD	ARG			20.351	20.897	42.683	1.00 40.90	
ATOM	844	NE	ARG			21.001	21.327	43.920	1.00 39.92	พ
ATOM	845	CZ	ARG	_		21.337	20.523	44.921	1.00 39.89	C
ATOM	846		ARG			21.084	19.217	44.856	1.00 39.37	N
ATOM	847		ARG			21.930	21.027	45.998	1.00 39.45	N
ATOM	848	N			121	15.769	20.109	44.115	1.00 39.00	N
ATOM	849	CA			121	15.380	18.956	44.908	1.00 40.44	C
ATOM	850	·C			121	15.840	17.702	44.161	1.00 39.32	c
ATOM	851	0			121	15.716	17.617	42.942	1.00 39.30	0
ATOM	852	СВ			121	13.866	18.950	45.170	1.00 39.20	C
ATOM	853	CG			121	13.369	17.698	45.876	1.00 39.97	c
ATOM	854	CD			121	12.136	17.928	46.731	1.00 40.42	c
ATOM	855		GLU			12.291	18.365	47.890	1.00 41.22	0
ATOM	856		GLU			11.016	17.645	46.259		
ATOM	857	N			122	16.414	16.752	44.889	1.00 42.21 1.00 38.78	O N
ATOM	858	CA			122	16.879	15.519			И
ATOM	859	C			122	15.760	14.523	44.285 44.374	1.00 38.34	C
ATOM	860	0			122	15.171	14.323		1.00 38.13	C
ATOM	861	CB			122	18.092	14.333	45.435 45.025	1.00 38.09 1.00 38.08	0
ATOM	862	CG			122	19.263	15.928	45.025	1.00 38.08	C
ATOM	863	CD			122	19.581	16.289	44.936	1.00 38.04	C
ATOM	864		GLU			19.763	15.364	42.667		C
111 OF1	504	- CH1	2110	-	144	15.703	10.304	42.00/	1.00 38.89	0

ATOM	865	OE2 G			19.627	17.501	43.183	1.00			.0
MOTA	866		ET A		15.434	13.879	43.265	1.00			N
ATOM	867	CA M	ET A	123	14.384	12.885	43.312	1.00		•	C.
MOTA	868		ET A		14.536	11.819	42.242	1.00			C
ATOM	869		ET A			11.876	41.387		37.04		0
MOTA	870	CB N	MET A	123	13.021	13.565	43.225		38.01		C
ATOM	871	CG N	MET A	123	12.798	14.318	41.946		39.05		С
MOTA	872		MET A		11.177	15.064	41.910		41.38		S
ATOM	873		ÆT A		11.489	16.589	42.818		41.39		С
ATOM	874		LYS A		13.675	10.820	42.332		37.17		N
MOTA	875	CA I	LYS A	124	13.692	9.715	41.401		36.98		C
MOTA	876		LYS A		12.802	10.098	40.238		36.81		С
ATOM	877		LYS A		11.814	10.813			36.91		0
MOTA	878		LYS A		13.213	8.434	42.087		36.82		C
MOTA	879	CG . I	LYS A	. 124	14.081	7.989	43.281		36.79		С
ATOM	880	CD :	LYS A	. 124	15.488	7.553	42.856		36.83		С
MOTA	881		LYS A		16.390	7.206	44.031		36.89		С
MOTA	882		LYS A		17.822	7.412	43.680		36.99		N
MOTA	883		PHE A		13.145	9.622	39.056		36.49		N
MOTA	884	CA	PHE A	125	12.416	10.031	37.885		36.33		С
ATOM	885		PHE A		10.926	9.861	38.074		36.45		С
ATOM	886		PHE P		10.143	10.743	37.732		36.30		0
MOTA	887		PHE A		12.879	9.270	36.665		36.24		C
MOTA	888		PHE A		12.555	9.967	35.407		36.21		C
MOTA	889	CD1	PHE A	A 125	13.403	10.936	34.924		35.98		C
MOTA	890		PHE A		11.374	9.714	34.743		36.15		С
MOTA	891	CE1	PHE A	A 125	13.108	11.616	33.794		36.07		C
MOTA	892	CE2	PHE A	A 125	11.073	10.390	33.597		36.71		C
MOTA	893	CZ		A 125	11.943	11.350	33.120		36.73		С
MOTA	894	N		A 126	10.527	8.733	38.640		36.80		N
MOTA	895	CA		A 126	9.111	8.492	38.845		36.98		C
MOTA	896	· C		A 126	8.547	9.560	39.772		37.20		C
MOTA	897	0		A 126	7.376	9.923	39.669		37.15		0
MOTA	898	CB		A 126	8.845	7.080	39.390		36.97		C
MOTA	899			A 126	8.990	6.946	40.877		36.62		C
MOTA	900			A 126	7.935	7.115	41.747		35.91	•	N
ATOM	901			A 126	10.058	6.618	41.644		36.38		C
MOTA	902	_		A 126	8.352	6.921			35.63		C
MOTA	903			A 126	9.636				35.43		N
MOTA	904			A 127	9.383				37.34		N
MOTA	905			A 127	8.912				37.55		C
MOTA	906			A 127		12.379			37.54		C
MOTA	907			A 127	7.657				37.36		0
MOTA	908			A 127	9.914				37.65		C
MOTA	909			A 127	10.155				37.89		C
MOTA	910			A 127	11.113				38.14		0
MOTA	911			A 127	12.330				37.77		
ATOM	912			A 127	10.649				38.86		0
MOTA	913			A 128	9.557				0 37.65		N
MOTA	914			A 128	9.393				0 37.81		C
MOTA	91			A 128	8.090				0 37.95		C 0
MOTA	91			A 128	7.280				0 37.90		
ATOM	91			A 128	10.578				0 37.88		C
MOTA	91			A 128	10.332				0 37.52		C
MOTA	91			A 128	10.088				0 36.94		C
ATOM	92			A 128	10.380				0 37.02		C
ATOM	92			A 128	9.876				0 37.09		C
MOTA	92			A 128	10.170				0 37.21		C
ATOM	92			A 128	9.917				0 37.15 0 38.00		И
MOTA	92			A 129	7.878				0 38.00		C
ATOM	92	5 CA	٧AL	A 129	6.71	12.45	36.87	J 1.U	0 20.10		C

ATOM	926	С	VAL	A	129		5.442	12.637	37.671	1.00 38.	24	С
ATOM	927		VAL				4.494	13.286	37.224	1.00 38.		ō
ATOM	928		VAL				6.705	11.050	36.268	1.00 38.		Ċ
ATOM	929	CG1					5.398	10.810	35.508	1.00 38.		č
ATOM	930	CG2					7.935	10.841	35.372	1.00 38.		Č
ATOM	931		GLU				5.430	12.038	38.854	1.00 38.		N
ATOM	932		GLU				4.289	12.115	39.745	1.00 38.		C
ATOM	933	C	GLU				4.025	13.578	40.083	1.00 38.		c
ATOM	934	0	GLU									
ATOM	935	CB					2.898	14.056	39.960	1.00 38.		0
			GLU				4.547	11.265	40.997	1.00 38.		C
MOTA	936	CG	GLU				4.404	9.763	40.745	1.00 39.		C
ATOM .	937	CD	GLU				5.160	8.897	41.740	1.00 39.		C
ATOM	938	OE1				•	5.551	9.403	42.815	1.00 40.		0
ATOM	939	OE2					5.355	7.697	41.441	1.00 40.		0
ATOM	940	. И	LYS				5.070	14.299	40.471	1.00 38.		N
MOTA	941	CA	LYS				4.908	15.707	40.787	1.00 38.		С
MOTA	942	С	LYS				4.290	16.431	39.598	1.00 38.		С
MOTA	943	0	LYS				3.393	17.252	39.769	1.00 38.		0
ATOM	944	CB	LYS				6.240	16.356	41.149	1.00 38.	58	С
MOTA	945	CG	LYS			•	6.440	16.666	42.625	1.00 38.	76	С
ATOM	946	CD	LYS				7.045	18.060	42.753	1.00 39.	73	С
ATOM	947	CE	LYS	A	131		7.756	18.316	44.070	1:00 40.	49	С
ATOM	948	NZ.	LYS	Α	131		8.117	19.772	44.197	1.00 40.	68	И
MOTA	949	N	LEU	Α	132		4.764	16.136	38.391	1.00 38.	84	N
ATOM	950	CA	LEU	Α	132		4.196	16.771	37.208	1.00 39.	.00	C
MOTA	951	C	LEU	Α	132		2.726	16.429	37.113	1.00 39.	11	C
MOTA	952	0	LEU	Α	132		1.903	17.287	36.810	1.00 39.	.20	. 0
MOTA	953	CB	LEU	Α	132		4.894	16.328	35.932	1.00 38.	96	C
ATOM	954	CG	LEU	A	132		6.287	16.899	35.723	1.00 39.		C
MOTA	955	CD1	LEU				6.870	16.389	34.429	1.00 39.		C
ATOM	956		LEU				6.261	18.421	35.709	1.00 40.		C
MOTA	957	N			133		2.396	15.170	37.367	1.00 39.		N
MOTA	958	CA			133		1.005	14.758	37.335	1.00 39.		Ċ
ATOM	959	C			133		0.172	15.523	38.370	1.00 39		Č
ATOM	960	0			133		-0.893	16.034	38.029	1.00 39		Č
ATOM	961	СВ			133		0.874	13.250	37.536	1.00 39		Č
ATOM	962	N			134		0.656	15.631	39.611	1.00 39		. N
ATOM	963	CA			134	•	-0.129	16.279	40.677	1.00 40		
ATOM	964	Ç			134		-0.437	17.732	40.379	1.00 40		Č
ATOM	965	ŏ			134		-1.543	18.211	40.623	1.00 40		Č
ATOM	966	CB			134		0.564	16.198	42.041	1.00 40		č
ATOM	967	CG		_	134		-0.348	16.660	43.182	1.00 41		č
ATOM	968				134		-1.301	17.421	42.910	1.00 43		č
ATOM	969				134		-0.212	16.312	44.378	1.00 44		Č
ATOM	970	N			135		0.545	18.438	39.846	1.00 40		1
MOTA	971	CA			135		0.350	19.836	39.556	1.00 40		·
ATOM	972	C			135		-0.719	19.973	38.500	1.00 40		Č
ATOM	973	Ö			135		-1.648	20.759	38.652	1.00 40		
ATOM	974	СВ			135		1.639	20.455	39.085	1.00 40		
ATOM	975				135		2.612	20.455	40.261	1.00 40		(
ATOM	976				135		1.358	21.817	38.507			
	977				135					1.00 40		(
ATOM ATOM	978						4.056	20.688	39.842	1.00 40		(
		N			136		-0.596	19.198	37.431	1.00 40		i
MOTA	979	CA			136		-1.586	19.248	36.376	1.00 39		C
MOTA	980	C			136		-2.956	19.094	37.000	1.00 39		C
MOTA	981	0			136		-3.795	19.991	36.921	1.00 39		C
MOTA	982	CB			136		-1.350	18.144	35.361	1.00 40		(
MOTA	983	N			137		-3.158	17.972	37.679	1.00 40		1
MOTA	984	CA			137		-4.486	17.630	38.164	1.00 40		(
MOTA	985	C			137		-4.995	18.683	39.114	1.00 40		(
ATOM	986	0	GLN	A	137		-6.170	19.046	39.068	1.00 40	.75	(

MOTA	987	CB (GLN A	137	-4.502	16.247	38.829	1.00 4	10.24		Ċ
ATOM	988	N .	ARG A	138	-4.116	19.200	39.959	1.00 4			N
MOTA	989	CA.	ARG A	138	-4.560	20.159	40.956	1.00 4			С
ATOM		C.	ARG A	138	-4.568	21.588	40.419	1.00 4	10.54		C .
ATOM		0	ARG A	138	-4.678	22.541	41.188	1.00 4			0
ATOM			ARG A		-3.692	20.069	42.207	1.00	40.43		С
ATOM			ARG A		-2.399	20.868	42.161	1.00	40.03		С
ATOM			ARG A		-1.541	20.546	43.346	1.00	39.94		С
ATOM			ARG A		-0.431		43.580	1.00	39.71		N
ATOM			ARG A		0.842		43.498	1.00	40.13		С
ATOM			ARG A		1.164		43.150	1.00	40.53		N
ATOM			ARG A		1.800		43.747	1.00			N
ATOM		N	GLY A		-4.471		39.102	1.00			N
ATOM	1000	CA	GLY A		-4.418		38.508	1.00			С
ATOM	1001	C	GLY A		-3.432		39.176	1.00			C
ATOM	1002	ō	GLY A		-3.616		39.110	1.00			Ο.
ATOM	1003	N	GLY A		-2.370		39.780	1.00			N
ATOM	1003	CA	GLY A		-1.425		40.519	1.00			С
MOTA	1005	C	GLY A		-0.69		39.602		40.40		C
ATOM	1005	0	GLY A		-0.78		38.383		40.79		Ö
ATOM	1007	N	GLU F		-0.01		40.167		40.10		N
	1007	CA	GLU F		0.80		39.371		40.01		C
MOTA			GLU A		2.30		39.458		39.64		Č
ATOM	1009	С		141	3.11		38.692		39.52		ŏ
ATOM	1010	0		4 141 4 141	0.58		39.796		40.20		č
ATOM	1011	CB			-0.71		39.315		41.00		č
ATOM	1012	CG		A 141	-0.71		37.800		42.10		č
ATOM	1013	CD		A 141			37.113		41.99		Ö
MOTA	1014		GLU Z		0.19		37.113		43.15		ő
ATOM	1015		GLU I		-1.99				39.25		N
MOTA	1016	N		A 142	2.67						C
MOTA	1017	CA		A 142	4.07				38.95		C
MOTA	1018	С		A 142	4.61				38.74		0
ATOM	1019	0		A 142	3.85				38.77		C
MOTA	1020	CB		A 142	4.22				38.95		C
MOTA	1021	CG		A 142	5.65				38.90		. C
MOTA	1022	CD	•	A 142	5.79				38.93	•	
ATOM	1023	OE1		A 142	4.83				39.58		0
ATOM	1024			A 142	6.88				38.74		0
MOTA	1025	N		A 143	5.91				38.39		N
MOTA	1026	CA		A 143	6.56				38.25		C
MOTA	1027	C		A 143	. 7.80				38.14		C
MOTA	1028	0		A 143					38.46		0
MOTA	1029	CB		A 143	7.04				38.26		C
MOTA	1030	CG		A 143	5.98				37.89		C
MOTA	1031	CD		A 143	6.60				37.35		С
ATOM	1032	NE		A 143	5.6				36.66		N
MOTA	1033	CZ		A 143	5.3				36.40	•	С
ATOM	1034	NH:	1 ARG	A 143					36.41		N
MOTA	1035	NH:	2 ARG	A 143	4.3				37.02		N
MOTA	1036	N	LEU	A 144	8.1				37.71		N
ATOM	1037	CA	LEU	A 144	9.3				37.57		С
ATOM	1038	С		A 144	10.1	81 22.31			37.33		С
MOTA	1039	0		A 144	9.7	10 22.46			37.31		0
ATOM	1040	CB	LEU	A 144	8.9	79 20.90	9 37.858		37.69		С
ATOM	1041	CG		A 144	7.9				38.31		С
ATOM	1042			A 144	7.6				39.02		С
ATOM	1043			A 144	8.5	51 21.32	7 40.263	3 1.00	37.91		С
ATOM	1044			A 145	11.4	60 22.09	8 36.528	3 1.00	37.01		N
ATOM	1045			A 145	12.3			7 1.00	36.87		С
ATOM	1046			A 145	13.3			1 1.00	36.85		С
ATOM	1047			A 145	14.1				36.51		0
		_									

ATOM	1048	СВ	TYR	Α	145		13.043	23.255	35.110	1.00	36.92		С
ATOM	1049	CG	TYR	Α	145		13.505	23.446	33.686		36.38		Č
ATOM	1050	CD1	TYR	Α	145		13.845	22.383	32.875		36.31		Ċ
MOTA	1051	CD2	TYR	Α	145		13.619	24.716	33.163		36.28		Ċ
ATOM	1052	CE1	TYR	A	145		14.278	22.590	31.582		36.21		Ċ
ATOM	1053		TYR				14.047	24.923	31.880		35.94		č
ATOM	1054	CZ	TYR				14.374	23.862	31.093		35.54		Č
MCTA	1055	ОН	TYR				14.789	24.081	29.799		36.13		Ö
MOTA	1056	N	LEU				13.378	19.736	35.218		37.06		N
ATOM	1057	CA	LEU				14.396	18.742	35.477		37.49		C
ATOM	1058	С	LEU				15.628	19.029	34.629		37.55		C
ATOM	1059	ō	LEU				15.532	19.241	33.427		37.33		0
ATOM	1060	СВ			146		13.877	17.341	35.173		37.69		
ATOM	1061	CG			146		14.919	16.233	35.349		37.95		C
ATOM	1062	CD1					14.234	14.916	35.567				C
ATOM	1063		LEU				15.849	16.133	34.151		37.66 39.00		C
ATOM	1064	N	GLN				16.786	18.993	35.269				C
ATOM	1065	CA	GLN				18.053				37.84		N
ATOM	1066	C			147			19.259	34.617		38.09		C
ATOM	1067	0			147		19.088	18.397	35.306		37.92		C
ATOM	1068	СВ					19.453	18.661	36.443		37.87		0
ATOM	1069				147		18.421	20.725	34.773		38.37		С
	_	CG			147		17.331	21.686	34.362		39.01		С
ATOM	1070	CD			147		17.867	23.064	34.191		39.92		С
ATOM	1071	OE1			147		17.149	23.955	33.772		42.51	•	0
ATOM	1072		GLN				19.137	23.253	34.520		40.24		N
ATOM	1073	N			148		19.576	17.385	34.601		37.81		N
MOTA	1074	CA			148	•	401100	16.377	35.196		37.57		С
MOTA	1075	С			148		21.325	15.744	34.176		37.68		С
ATOM	1076	0			148		20.876	15.266	33.146		37.30		0
MOTA	1077	CB			148		19.576	15.261	35.773	1.00	37.61		С
ATOM	1078	CG			148		20.336	13.971	36.068	1.00	36.79		С
ATOM	1079	CD			148		21.398	14.159	37.117	1.00	35.97		С
ATOM	. 1080	OE1			148		21.162	14.814	38.135		35.11		0
MOTA	1081		GLN				22.577	13.593	36.875	1.00	35.03		N
MOTA	1082	N			149		22.596	15.698	34.503	1.00	38.15		N
MOTA	1083	CA			149		23.574	15.130	33.622	1.00	38.57		С
MOTA	1084	С	THR	Α	149		23.354	13.647	33.506	1.00	38.68		С
MOTA	1085	Ö	THR	Α	149		23.154	12.973	34.509	1.00	39.07		0
ATOM	1086	CB	THR	A	149		24.936	15.410	34.214	1.00	38.75		С
ATOM	1087		THR				25.206	16.807	34.088	1.00	38.86	•	0
MOTA	1088	CG2	THR	Α	149		26.036	14.759	33.418	1.00	39.39		. C
MOTA	1089	N	LEU	Α	150		23.393	13.144	32.279		38.87		N
MOTA	1090	CA	LEU	Α	150		23.259	11.722	32.021		39.24		C
MOTA	1091	С	LEU	A	150		24.498	10.979	32.507		39.20		Ċ
ATOM	1092	0			150		25.602	11.317	32.101		39.20		ő
ATOM	1093	CB			150		23.146	11.465	30.519		39.46	•	č
MOTA	1094	CG			150		21.938	11.942	29.722		40.52		č
ATOM	1095	CD1	LEU				22.077	11.563	28.237		41.06		Č
ATOM	1096		LEU				20.712	11.308	30.303		41.66		Č
ATOM	1097	N			151		24.315	9.960	33.343		39.19		N
MOTA	1098	CA			151		25.436	9.171	33.861		39.46		c
MOTA	1099	С			151		25.193	7.642	33.883		39.43		č
ATOM	1100	Ō			151		24.198	7.162	33.333		39.15		0
ATOM	1101	СВ			151		25.731	9.652	35.265		39.54		
ATOM	1102	CG			151		24.511	9.588	36.150		40.08	٠-	C
ATOM	1103		ASN				23.874	8.533	36.283				C
ATOM	1104		ASN				24.158	10.725			39.68		0
ATOM	1105	ND2			152		26.075		36.751		40.83		N
ATOM	1105	CA			152		26.075	6.892	34.556		39.43		N
ATOM	1100	CA			152			5.413	34.543		39.58		C
ATOM	1107	0			152		24.761	4.787	35.083		39.17		C
ALOR	1100	J	MOL	A	132		24.477	3.634	34.776	1.00	39.29		0

ATOM	1109	CB .	ASP A 152	27.138	4.756	35.385	1.00 39.92		С
ATOM	1110	CG .	ASP A 152	28.489	5.382	35.198	1.00 41.53		С
ATOM	1111		ASP A 152	28.722	6.005	34.134	1.00 45.10		0
ATOM	1112		ASP A 152	29.378	5.294	36.076	1.00 42.02		0
ATOM	1113		THR A 153	24.008	5.493	35.909	1.00 38.78		N
ATOM	1114		THR A 153	22.881	4.830	36.542	1.00 38.50		С
ATOM	1115		THR A 153	21.757	4.573	35.573	1.00 38.26		C
ATOM	1116		THR A 153	20.842	3.838	35.882	1.00 38.29		0
ATOM	1117		THR A 153	22.329	5.624	37.733	1.00 38.46	•	Č
ATOM	1118		THR A 153	21.622	6.780	37.269	1.00 39.25		Ö
ATOM	1119		THR A 153	23.445	6.161	38.611	1.00 38.28		č
ATOM	1120		VAL A 154	21.804	5.165	34.396	1.00 38.28		N
ATOM	1121	CA	VAL A 154	20.687	4.977	33.491	1.00 38.29		Ċ
ATOM	1122		VAL A 154	20.602	3.530	33.067	1.00 38.17		Ċ
ATOM	1123	0	VAL A 154	21.597	2.805	33.092	1.00 38.10		ŏ
	1123	СВ	VAL A 154	20.786	5.838	32.251	1.00 38.15		č
MOTA	1125		VAL A 154	20.815	7.291	32.649	1.00 38.22		c
ATOM				22.007	5.437	31.443	1.00 38.40		C
ATOM	1126		VAL A 154				1.00 38.40		N
ATOM	1127	N	GLY A 155	19.395	3.132	32.681	1.00 38.03		C
ATOM	1128	CA	GLY A 155	19.114	1.779	32.258			C
MOTA	1129	C	GLY A 155	19.609	1.358	30.894	1.00 38.17		
ATOM	1130	0	021 11 100	20.092	2.153	30.081	1.00 38.44		0
ATOM	1131	N	ARG A 156	19.417	0.073	30.642	1.00 38.16		И
MOTA	1132	CA	ARG A 156	19.932	-0.588	29.461	1.00 38.16		C
ATOM	1133	C	ARG A 156	19.414	0.065	28.210	1.00 38.01		C
MOTA	1134	0	ARG A 156	20.185	0.490	27.346	1.00 38.04		0
MOTA	1135	CB	ARG A 156	19.554	-2.080	29.489	1.00 38.18		C
MOTA	1136	N	LYS A 157	18.102	0.178	28.118	1.00 37.83		N
MOTA	1137	CA	LYS A 157	17.545	0.713	26.905	1.00 37.67		· C
MOTA	1138	С	LYS A 157	18.144	2.092	26.679	1.00 37.77		С
MOTA	1139	0	LYS A 157	18.579	2.386	25.571	1.00 37.84		0
MOTA	1140	CB	LYS A 157	16.014	0.725	26.936	1.00 37.62		С
ATOM	1141	CG	LYS A 157	15.379	-0.624	26.550	1.00 36.92		С
MOTA	1142	N	ILE A 158	18.247	2.911	27.728	1.00 · 37.82		N
ATOM	1143	CA	ILE A 158	18.699	4.287	27.526	1.00 37.81		С
MOTA	1144	С	ILE A 158	20.096	4.252	27.008	1.00 37.78		C
MOTA	1145	0	ILE A 158	20.440	4.942	26.058	1.00 37.52		0
MOTA	1146	CB	ILE A 158		5.109	28.802	1.00 37.90		С
MOTA	1147	CG1	ILE A 158		5.283	29.280	1.00 37.87		С
ATOM	1148	CG2	! ILE A 158	19.281	6.477	28.538	1.00 37.57		С
ATOM	1149	CD1	ILE A 158		6.034	28.318	1.00 37.95		С
ATOM	1150	N	VAL A 159	20.899	3.418	27.637	1.00 37.89		N
MOTA	1151	CA	VAL A 159	22.263	3.265	27.211	1.00 38.06		С
MOTA	1152	С	VAL A 159	22.255	2.906	25.725	1.00 38.07		С
ATOM	1153	0	VAL A 159	· 23.025	3.462	24.955	1.00 37.93		0
MOTA	1154	CB	VAL A 159		2.196	28.039	1.00 38.12		С
MOTA	1155		L VAL A 159		1.740	27.315	1.00 38.65		С
MOTA	1156		2 VAL A 159		2.734	29.410	1.00 37.65		С
ATOM	1157		MET A 160		1.984	25.318	1.00 38.30		N
ATOM	1158				1.658	23.894	1.00 38.71		С
ATOM	1159		MET A 160		2.923			•	С
ATOM	1160		MET A 160		3.219				0
ATOM	1161				0.682				Ċ
ATOM	1162				-0.690				c
ATOM	1163				-1.293				s
MOTA	1163				-1.709				c
ATOM	1165		ASP A 161		3.665				N
ATOM	1166				4.902				. C
MOTA			ASP A 161		5.788				C
	1167		ASP A 161		6.154				0
ATOM ATOM	1168 1169				5.650				C
MIOM	1102	, (5	WAL W TO	10.031	3.030	~J.J.L	1.00 37.04		C

MOTA	1170	CG :	ASP A 1	61	17.274	4.908	23.501	1.00 3	37.82	С
ATOM	1171		ASP A 1		17.082	4.020	22.646	1.00 3		0
MOTA	1172		ASP A 1		16.366	5.155	24.320	1.00 3	38.41	0
MOTA	1173		PHE A 1		21.539	6.100	23.836	1.00 3	36.93	N
MOTA	1174		PHE A 1		22.672	7.020	23.919	1.00 3	36.54	С
MOTA	1175		PHE A 1		23.760	6.604	22.960	1.00 3		C
MOTA	1176		PHE A 1		24.375	7.446	22.304	1.00 3	36.06	0
MOTA	1177		PHE A 1		23.201	7.063	25.364	1.00 3	36.52	C
MOTA	1178		PHE A 1		24.386	7.974	25.576	1.00 3	36.64	C
MOTA	1179		PHE A 1		24.209	9.319	25.871	1.00	36.67	C
ATOM	1180		PHE A 1		25.682	7.467	25.540	1.00	37.81	С
ATOM	1181		PHE A 1		25.299	10.155	26.081	1.00	36.91	С
MOTA	1182		PHE A 1		26.787	8.300	25.764	1.00	37.75	С
MOTA	1183	CZ	PHE A 1		26.592	9.640	26.029	1.00	37.82	С
MOTA	1184	N	LEU A 1		23.976	5.297	22.878	1.00	35.38	N
MOTA	1185	CA	LEU A 1		24.998	4.730	22.023	1.00	34.93	С
MOTA	1186	С	LEU A 1		24.635	4.948	20.591		34.41	С
MOTA	1187	0	LEU A 1		25.502	5.067	19.732		34.36	0
MOTA	1188	CB	LEU A 1		25.111	3.239	22.272	1.00	35.05	С
MOTA	1189	CG	LEU A 1		25.977	2.932	23.473		35.25	С
MOTA	1190		LEU A 1		.25.944	1.471	.23.684	1.00	36.00	С
MOTA	1191	CD2	LEU A 1		27.404	3.425	23.270	1.00	35.64	C
MOTA	1192	N	GLY A 1	L64	23.336	4.977	20.338	1.00	33.85	N
MOTA	1193	CA	GLY A		22.832	5.230	19.009	1.00	33.55	C
MOTA	1194	C	GLY A		22.874	6.682	18.548	1.00	33.11	C
MOTA	1195	0	GLY A		22.361	6.977	17.471	1.00		0
MOTA	1196	N	PHE A		23.443	7.589	19.341		32.16	N
ATOM	1197	CA	PHE A		23.593	8.964	18.894	1.00		С
MOTA	1198	C	PHE A		24.628	8.972	17.752	1.00	30.93	С
MOTA	1199	0	PHE A		25.413	8.063	17.650		30.67	0
MOTA	1200	·CB	PHE A		24.028	9.883	20.055		32.06	С
MOTA	1201	CG	PHE A		22.989	10.052	21.160		32.55	С
MOTA	1202		PHE A		21.734	9.478	21.081		33.69	С
ATOM	1203	CD2			23.293	10.786	22.289		32.64	С
MOTA	1204		PHE A		20.817	9.646	22.106		33.39	С
MOTA	1205		PHE A		22.380	10.948	23.308		32.11	. C
MOTA	1206	CZ	PHE A		21.150	10.380	23.218		32.69	С
MOTA	1207	N	ASN A		24.600	9.977	16.881		30.43	N
ATOM	1208	CA	ASN A		25.552	10.106	15.761		30.00	C
ATOM	1209	C	ASN A		26.932	10.623	16.177		29:91	C
ATOM	1210	0	ASN A		27.370	11.721	15.812		28.90	0
ATOM	1211	CB	ASN A		24.957	11.013	14.673		29.86	C
ATOM	1212	CG	ASN A		25.720	10.957	13.363		28.91	C
MOTA	1213		ASN A		26.836	10.423	13.282		27.68	0
ATOM	1214		ASN A		25.119	11.528	12.320		26.76	N
MOTA	1215	N	TRP A		27.604	9.785	16.943		30.04	N
ATOM	1216	CA	TRP A		28.938	10.044	17.399		30.41	C
ATOM	1217	С	TRP A		29.823	10.295	16.205		30.80	C
ATOM	1218	0	TRP A		30.708	11.141	16.237		30.55	0
MOTA	1219	CB	TRP A		29.390	8.847	18.232		30.31	C
MOTA	1220	CG	TRP A		28.513	8.746	19.433		30.59	C
MOTA	1221		TRP A		27.594	7.792	19.699		30.51	C
ATOM	1222	CD2			28.422	9.696	20.502		31.94	C
MOTA	1223		TRP A		26.947	8.067	20.881		30.98	И
ATOM	1224		TRP A		27.442	9.232	21.395		31.41	C
ATOM	1225	CE3			29.087	10.885	20.801		31.71	C
ATOM	1226		TRP A		27.112	9.904	22.554		32.59	C
MOTA	1227		TRP A		28.750	11.560	21.944		32.92	C
ATOM	1228	CH2			27.773	11.072	22.811		33.34	C
ATOM	1229		ASN A		29.549	9.596	15.119		31.69	N
ATOM	1230	CA	ASN A	тря	30.352	9.771	13.936	T.00	32.37	C

MOTA	1231 C ASN A 168	30.447 11.229 13.590 1.00 32.97
MOTA	1232 O ASN A 168	31.541 11.747 13.390 1.00 33.15
ATOM	1233 CB ASN A 168	29.729 9.064 12.749 1.00 32.68
ATOM	1234 CG ASN A 168	30.594 9.147 11.507 1.00 32.86
MOTA	1235 OD1 ASN A 168	31.797 8.914 11.574 1.00 35.02
ATOM	1236 ND2 ASN A 168	29.989 9.473 10.368 1.00 31.39
ATOM	1237 N TRP A 169	29.284 11.884 13.518 1.00 33.38
MOTA	1238 CA TRP A 169	29.200 13.279 13.107 1.00 33.28
ATOM	1239 C TRP A 169	29.711 14.237 14.149 1.00 33.33
	1240 O TRP A 169	30.406 15.188 13.834 1.00 33.43
MOTA		27.756 13.673 12.765 1.00 33.43
MOTA		27.618 15.134 12.412 1.00 33.11
MOTA	1242 CG TRP A 169	27.814 15.698 11.191 1.00 33.49
MOTA	1243 CD1 TRP A 169	- · · · · · · · · · · · · · · · · · · ·
MOTA	1244 CD2 TRP A 169	
MOTA	1245 NE1 TRP A 169	
MOTA	1246 CE2 TRP A 169	
MOTA	1247 CE3 TRP A 169	
ATOM	1248 CZ2 TRP A 169	27.026 18.648 13.081 1.00 33.66
MOTA	1249 CZ3 TRP A 169	26.719 17.526 15.204 1.00 34.02
ATOM	1250 CH2 TRP A 169	26.733 18.695.14.413 1.00 34.21
MOTA	1251 N ILE A 170	29.369 14.021 15.398 1.00 33.54
ATOM	1252 CA ILE A 170	29.739 15.024 16.368 1.00 33.92
ATOM	1253 C ILE A 170	31.225 14.935 16.713 1.00 34.07
ATOM	1254 O ILE A 170	31.855 15.939 16.988 1.00 34.23
MOTA	1255 CB ILE A 170	28.832 14.947 17.591 1.00 33.84
ATOM	1256 · CG1 ILE A 170	28.803 16.288 18.306 1.00 34.22
ATOM	1257 CG2 ILE A 170	29.295 13.858 18.499 1.00 34.45
	1257 CG2 1111 11 170	27.869 16.309 19.478 1.00 34.73
MOTA	1259 N ASN A 171	31.801 13.743 16.650 1.00 34.41
ATOM		33.222 13.593 16.950 1.00 34.46
ATOM		34.055 14.322 15.918 1.00 34.56
MOTA	1261 C ASN A 171	
MOTA	1262 O ASN A 171	
ATOM	1263 CB ASN A 171	
MOTA	1264 CG ASN A 171	
MOTA	1265 OD1 ASN A 171	
MOTA	1266 ND2 ASN A 171	
ATOM	1267 N LYS A 172	
MOTA	1268 CA LYS A 172	34.337 14.917 13.584 1.00 35.18
MOTA	1269 C LYS A 172	34.261 16.415 13.907 1.00 35.29
MOTA	1270 O LYS A 172	35.248 17.133 13.800 1.00 34.89
ATOM	1271 CB LYS A 172 .	
ATOM	1272 CG LYS A 172	34.200 13.299 11.587 1.00 36.55
ATOM	1273 CD LYS A 172	33.873 13.158 10.090 1.00 38.20
ATOM	1274 CE LYS A 172	34.512 11.872 9.537 1.00 39.82
MOTA		34.369 11.661 8.050 1.00 41.20
ATOM		33.093 16.875 14.339 1.00 35.70
· ATOM		32.931 18.272 14.699 1.00 36.20
ATOM		33.929 18.633 15.771 1.00 36.47
ATOM		34.605 19.656 15.686 1.00 36.97
ATOM		31.534 18.555 15.231 1.00 36.19
ATOM		30.473 18.637 14.167 1.00 36.97
ATOM		30.765 19.720 13.157 1.00 37.19
ATOM		31.198 20.808 13.531 1.00 38.68
ATOM		30.551 19.425 11.879 1.00 35.94
		34.000 17.806 16.802 1.00 36.38
ATOM		34.945 18.041 17.866 1.00 36.42
ATOM		36.360 18.102 17.283 1.00 36.56
ATOM		37.161 18.945 17.672 1.00 36.42
ATOM		34.815 16.937 18.912 1.00 36.33
MOTA		35.896 16.908 19.963 1.00 36.13
OTA		
1OTA	4 1291 CD GLN A 174	35.785 15.676 20.815 1.00 36.16

ATOM	1292		GLN			35.415	14.613	20.314	1.00 37.84		0
MOTA	1293	NE2	GLN	A	174	36.082	15.803	22.103	1.00 34.98		N
MOTA	1294	N	GLY			36.649	17.231	16.322	1.00 36.76		N
MOTA	1295	CA	GLY			37.976	17.158	15.750	1.00 36.97		С
ATOM	1296	С	GLY			38.302	18.356	14.892	1.00 37.21		C
ATOM	1297	0	GLY			39.336	18.993	15.070	1.00 37.38		0
ATOM	1298	N	LYS			37.406	18.682	13.971	1.00 37.44		N
MOTA	1299	CA	LYS			37.634	19.793	13.064	1.00 37.56		С
ATOM ATOM	1300 1301	C	LYS			37.898	21.090	13.822	1.00 37.47	-	С
ATOM	1301	O CB	LYS			38.713	21.907	13.400	1.00 37.47		0
ATOM	1302	CG	LYS LYS			36.423	20.014	12.161	1.00 37.71		C
	1303	CD	LYS			36.134 34.960	18.905 19.284	11.163	1.00 38.70		C
ATOM	1305	CE	LYS			34.064	18.092	10.279 10.037	1.00 39.76 1.00 41.48		C
MOTA	1306	NZ			176	32.663	18.481	9.690	1.00 41.48		C
ATOM	1307	N	ARG			37.212	21.283	14.938	1.00 43.43		N N
ATOM	1308	CA	ARG			37.325	22.544	15.643	1.00 37.10		C
ATOM	1309	С	ARG			38.352	22.495	16.763	1.00 36.85	•	C
ATOM	1310	0	ARG			38.445	23.420	17.564	1.00 36.21		ō
ATOM	1311	CB	ARG	Α	177	35.980	22.969	16.228	1.00 37.21		Č
MOTA	1312	CG	ARG	A	177	34.807	22.773	15.326	1.00 37.50		C
MOTA	1313	CD	ARG			34.802	23.591	14.053	1.00 38.49		C
ATOM	1314	NE			177	33.750	23.066	13.185	1.00 39.56		N
ATOM	1315	CZ			177	33.884	22.803	11.891	1.00 41.17		С
ATOM	1316	NH1				35.026	23.050	11.254	1.00 41.34		И
ATOM	1317		ARG			32.855	22.304	11.219	1.00 41.89		N
ATOM	1318	N			178	39.088	21.401	16.859	1.00 36.70		N
ATOM ATOM	1319 1320	CA			178	40.131	21.337	17.854	1.00 36.74		C
ATOM	1321	C O			178 178	39.592	21.509	19.249	1.00 36.76		C
ATOM	1322	N			178	40.340	21.817	20.171	1.00 37.18		0
ATOM	1323	CA			179	38.293 37.722	21.331 21.439	19.420	1.00 36.75		N
ATOM ·	1324	C			179	38.309	20.400	20.745 21.679	1.00 36.66 1.00 36.60		C
ATOM	1325	ŏ			179	38.980	19.451	21.260	1.00 36.60 1.00 35.99		C
ATOM	1326	CB			179	36.222	21.216	20.708	1.00 36.79		0
ATOM	1327	CG			179	35.454	22.258	20.038	1.00 36.73		C
ATOM	1328	CD1			179	35.889	23.470	19.620	1.00 36.67		c
MOTA	1329	CD2			179	34.081	22.180	19.692	1.00 37.40		Č
MOTA	1330	NE1			179	34.860	24.168	19.035	1.00 36.91		N
MOTA	1331	CE2			179	33.735	23.390	19.062	1.00 37.43	•	C
MOTA	1332	CE3			179	33:099	21.198	19.840	1.00 36.64		С
ATOM	1333		TRP			32.456	23.641	18.583	1.00 36.83		С
ATOM	1334		TRP			31.840	21.450	19.365	1.00 36.84		С
ATOM ATOM	1335 1336		TRP			31.524	22.661	18.744	1.00 36.02		C
ATOM	1337	N CA			180	38.022	20.595	22.958	1.00 36.66		N
ATOM	1338	C			180 180	38.444	19.681	23.992	1.00 36.96		C
ATOM	1339	Ö			180	37.456 36.698	18.548	24.131	1.00 37.25		C
ATOM	1340	N			181	37.445	18.285 17.891	23.204 25.288	1.00 37.69		0
ATOM	1341	CA			181	36.581	16.734	25.507	1.00 37.46 1.00 37.81		И
MOTA	1342	C			181	35.136	17.088	25.802	1.00 37.81		C
MOTA	1343	0			181	34.825	18.177	26.273	1.00 37.40		0
MOTA	1344	CB			181	37.082	15.881	26.680	1.00 37.33		C
ATOM	1345	CG			181	36.684	16.433	28.065	1.00 30.10		C
ATOM	1346	CD	GLN	Α	181	36.956	15.470	29.231	1.00 43.44		C
MOTA	1347		GLN	A	181	38.004	14.802	29.284	1.00 44.84		ŏ
MOTA	1348	NE2	GLN	A	181	36.007	15.406	30.173	1.00 44.80		N
MOTA	1349	N _.			182	34.266	16.130	25.510	1.00 37.00		N
MOTA	1350	CA			182	32.866	16.181	25.878	1.00 36.47		С
ATOM	1351	C			182	32.856	16.224	27.385	1.00 35.97		С
ATOM	1352	0	TEO	A	182	33.345	15.298	28.009	1.00 35.98		0

MOTA	1353	CB LEU A 182				1.00 36.38
ATOM	1354	CG LEU A 182	30.691	14.707		1.00 36.76
ATOM	1355	CD1 LEU A 182	30.339	13.254		1.00 36.70
MOTA	1356	CD2 LEU A 182	29.917	15.417		1.00 37.66
ATOM	1357	N THR A 183	32.337	17.270		1.00 35.50
MOTA	1358	CA THR A 183	32.310	17.230	29.457	1.00 35.07
ATOM	1359	C THR A 183	31.008	16.669	29.929	1.00 34.39
MOTA	1360	O THR A 183	30.944	16.097	31.000	1.00 34.13
	1361	CB THR A 183	32.528	18.599	30.105	1.00 35.07
ATOM		OG1 THR A 183	31.402	19.444	29.883	1.00 35.21
ATOM	1362	CG2 THR A 183	33.652	19.310	29.453	1.00 35.76
MOTA	1363		29.947.	16.848	29.163	1.00 33.83
ATOM	1364	N SER A 184		16.288	29.626	1.00 33.03
MOTA	1365	CA SER A 184	28.710		28.684	1.00 33.13
MOTA	1366	C SER A 184	27.563	16.459	27.699	1.00 32.72
ATOM	1367	O SER A 184	27.643	17.172		1.00 32.39
ATOM	1368	CB SER A 184	28.363	16.954	30.949	
MOTA	1369	OG SER A 1.84	28.349	18.347	30.788	1.00 31.82
MOTA	1370	N ASN A 185	26.484	15.776	29.013	1.00 32.44
ATOM	1371	CA ASN A 185	25.259	15.893	28.277	1.00 32.59
MOTA	1372	C ASN A 185	24.218	16.117	29.319	1.00 33.00
ATOM	1373	O ASN A 185	24.027	15.285	30.184	1.00 32.72
ATOM ·	1374	CB ASN A 185	24.917	14.619	27.520	1.00 32.46
MOTA	1375	CG ASN A 185	25.850	14.351	26.369	1.00 31.69
ATOM	1376	OD1 ASN A 185	26.661	13.436	26.434	1.00 32.60
ATOM	1377	ND2 ASN A 185	25.725	15.121	25.297	1.00 29.86
ATOM	1378	N LEU A 186	23.549	17.252	29.258	1.00 33.80
ATOM	1379	CA LEU A 186	22.537	17.536	30.241	1.00 34.36
ATOM	1380	C LEU A 186	21.199	17.117	29.684	1.00 34.78
ATOM	1381	O LEU A 186	20.903	17.380	28.512	1.00 35.02
ATOM	1382	CB LEU A 186	22.500	19.029	30.539	1.00 34.34
	1383	CG LEU A 186	21.564	19.433	31.677	1.00 35.25
MOTA	1384	CD1 LEU A 186	22.122	18.827	32.930	1.00 35.58
ATOM		CD2 LEU A 186	21.402	20.956	31.845	1.00 35.43
ATOM	1385		20.393	16.456	30.507	1.00 34.95
ATOM	1386		19.022	16.189	30.120	1.00 35.27
MOTA	1387			17.260	30.735	1.00 35.48
MOTA	1388		18.117		31.951	1.00 35.40
ATOM	1389		18.105	17.449		1.00 35.40
MOTA	1390		18.593	14.805		1.00 35.33
MOTA	1391		17.105	14.481		1.00 36.40
MOTA	1392		16.624		28.969 30.940	
MOTA	1393		16.850	13.114		1.00 36.96
MOTA	1394			17.977		
MOTA	1395		16.466			1.00 35.89
MOTA	1396		15.047			1.00 36.32
MOTA	1397		14.738			1.00 36.89
MOTA			16.795			1.00 35.79
MOTA			18.210			1.00 35.66
MOTA	1400	CD1 LEU A 188 ·	18.976			1.00 36.04
MOTA	1401		18.125			1.00 35.23
ATOM	1402	2 N ILE A 189	14.184			
MOTA		3 CA ILE A 189	12.782			
MOTA			12.105	19.353		
ATOM			12:388			
ATOM			12.368	16.916		
ATOM		-	13.126			
ATOM			10.865		31.143	
ATOM			12.884			1.00 36.11
ATOM			11.221			1.00 35.53
ATOM			10.614			
ATOM			9.184			
ATOM			8.748			
AION						

ATOM	1414	N	MET .	A	191		8.458	22.208	31.696	1.00 35.18	N
ATOM	1415	CA	MET .	A	191		7.063	22.463	31.447	1.00 35.16	С
MOTA	1416	С	MET .				6.916	23.584	30.446	1.00 35.00	С
MOTA	1417	0	MET .		-		7.795	24.426	30.316	1.00 35.17	0
ATOM	1418	CB	MET				6.379	22.849	32.750	1.00 35.13	С
MOTA	1419	CG ·	MET				6.277	21.691	33.710	1.00 35.63	C
MOTA	1420	SD	MET				5.756	22.150	35.360	1.00 35.65	S
ATOM	1421	CE	MET				4.222	22.827	35.017	1.00 36.16	C
ATOM ATOM	1422 1423	N CA	GLU GLU				5.804 5.492	23.573 24.626	29.727 28.791	1.00 34.83	И
ATOM	1423	CA	GLU				5.585	25.955	29.511	1.00 34.74 1.00 34.72	C
MOTA	1425	o	GLU				5.184	26.067	30.674	1.00 34.72	0
ATOM	1426	СВ	GLU				4.085	24.447	28.264	1.00 34.75	Č
ATOM	1427	CG	GLU				3.029	24.525	29.348	1.00 35.09	Ċ
MOTA	1428	CD	GLU				1.669	24.117	28.842	1.00 34.97	, Č
ATOM	1429	OE1	GLU				1.609	23.503	27.756	1.00 33.58	. 0
MOTA	1430	OE2	GLU				0.672	24.422	29.530	1.00 35.72	0
MOTA	1431	N	GLY				6.121	26.953	28.818	1.00 34.53	N
MOTA	1432	CA	GLY				6.265	28.279	29.378	1.00 34.63	С
MOTA	1433	С	GLY				7.528	28.542	30.180	1.00 34.49	
MOTA	1434	0	GLY				7.864	29.694	30.434	1.00 34.57	
MOTA	1435	N	ASN				8.224	27.493	30.594	1.00 34.27	
ATOM	1436	CA	ASN			_	9.441	27.672	31.367	1.00 34.06	
MOTA	1437	С	ASN				10.466	28.492	30.609	1.00 33.93	
MOTA MOTA	1438 1439	O CB	ASN ASN				10.552 10.051	28.415 26.316	29.392 31.721	1.00 33.84 1.00 33.99	
ATOM	1440	CG	ASN			•	9.314	25.625	32.836	1.00 33.99	
ATOM	1441		ASN				8.257	26.081	33.265	1.00 33.13	
ATOM	1442		ASN				9.869	24.528	33.323	1.00 31.93	
ATOM	1443	N	VAL			:	11.243	29.285	31.332	1.00 33.86	
MOTA	1444	CA			195		12.288	30.069	30.707	1.00 33.70	
MOTA	1445	С			195		13.621	29.969	31.396	1.00 33.38	
MOTA	1446	0			195	:	13.721	30.115	32.601	1.00 33.75	
MOTA	1447	CB			195		11.964	31.552	30.779	1.00 33.96	
ATOM	1448	CG1					13.151	32.389	30.253	1.00 34.32	
MOTA	1449		VAL				10.693	31.854	30.032	1.00 34.15	
ATOM	1450	N			196		14.666	29.764	30.621	1.00 33.04	
ATOM	1451	CA			196	•	15.991	29.883	31.161	1.00 32.60	
MOTA MOTA	1452 1453	C 0			196 196		16.438	31.256	30.723	1.00 32.21	
ATOM	1454	СВ			196		16.584 16.887	31.500 28.836	29.530 30.586	1.00 31.64	
ATOM	1455		THR				16.466	27.543	31.048	1.00 32.00	
ATOM	1456		THR				18.281	29.003	31.124	1.00 32.63	
ATOM	1457	N			197		16.585	32.177	31.672	1.00 31.97	
MOTA	1458	CA			197		17.000	33.530	31.350	1.00 31.74	
MOTA	1459	С			197		18.385	33.564	30.816	1.00 31.92	
MOTA	1460	0	PRO	A	197		19.215	32.717	31.129	1.00 32.52	
MOTA	1461	CB			197		16.950	34.234	32.682	1.00 31.38	3 C
MOTA	1462	CG			197		16.056	33.508	33.418	1.00 31.84	
ATOM	1463	CD			197		16.305	32.055	33.107	1.00 32.08	
ATOM	1464	N			. 198		18.615	34.592	30.024	1.00 32.00	
ATOM	1465	CA			198		19.846	34.787	29.311	1.00 32.28	
MOTA	1466	C			198		21.101	34.690	30.162		
ATOM ATOM	1467 1468	O CB			198 198		21.213 19.798	35.305 36.131	31.220		
ATOM	1469	N			198		22.064	33.953	28.625 29.630	1.00 32.42 1.00 32.73	
ATOM	1470	. CA			. 199 . 199		23.339	33.737	30.271		
MOTA	1471	C			199		24.308	33.252	29.220		
MOTA	1472	Ö			199		23.902	33.013	28.084	1.00 33.70	
MOTA	1473	СВ			199		23.194	32.622	31.275	1.00 33.24	
ATOM	1474	CG			199		22.879	31.311	30.639		

MOTA	1475 ND1 HIS A 199	21.602 30.958 30.269 1.00 31.40
ATOM	1476 CD2 HIS A 199	23.679 30.292 30.253 1.00 32.85
MOTA	1477 CE1 HIS A 199	21.624 29.761 29.714 1.00 32.37
ATOM	1478 NE2 HIS A 199	22.871 29.330 29.698 1.00 32.78
ATOM	1479 N TYR A 200	25.575 33.093 29.601 1.00 34.35
ATOM	1480 CA TYR A 200	26.580 32.502 28.712 1.00 34.92
ATOM	1481 C TYR A 200	27.256 31.350 29.431 1.00 35.15
ATOM	1482 O TYR A 200	27.285 31.318 30.661 1.00 35.76
		27.599 33.510 28.175 1.00 34.90
ATOM		28.586 34.096 29.156 1.00 34.89
ATOM		29.825 33.519 29.359 1.00 33.02
MOTA		28.307 35.292 29.802 1.00 36.04
ATOM	1486 CD2 TYR A 200	
MOTA	1487 CE1 TYR A 200	
MOTA	1488 CE2 TYR A 200	
MOTA	1489 CZ TYR A 200	30.410 35.253 30.882 1.00 34.40
ATOM	1490 OH TYR A 200	31.301 35.855 31.739 1.00 32.62
MOTA	1491 N ASP A 201	27.747 30.387 28.654 1.00 35.04
MOTA	1492 CA ASP A 201	28.386 29.189 29.182 1.00 34.82
MOTA	1493 C ASP A 201	29.818 29.220 28.652 1.00 34.87
ATOM	1494 O ASP A 201	30.047 29.734 27.588 1.00 34.81
MOTA	1495 CB ASP A 201	27.636 27.925 28.727 1.00 34.49
ATOM	1496 CG ASP A 201	26.212 27.854 29.256 1.00 34.63
MOTA	1497 OD1 ASP A 201	26.046 27.953 30.480 1.00 33.52
ATOM	1498 OD2 ASP A 201	25.191 27.680 28.533 1.00 36.84
ATOM	1499 N GLU A 202	30.795 28.727 29.399 1.00 35.74
MOTA	1500 CA GLU A 202	32.176 28.699 28.899 1.00 36.38
ATOM	1501 C GLU A 202	
MOTA	1502 O GLU A 202	33.679 27.019 28.126 1.00 37.04
ATOM	1503 CB GLU A 202	33.172 28.830 30.048 1.00 36.61
ATOM	1504 CG GLU A 202	33.100 30.185 30.725 1.00 37.81
ATOM	1505 CD GLU A 202	33.960 30.276 31.949 1.00 38.93
	1506 OE1 GLU A 202	33.525 29.783 33.020 1.00 39.85
MOTA	1507 OE2 GLU A 202	35.055 30.858 31.832 1.00 40.19
MOTA		31.556 26.840 27.462 1.00 35.68
ATOM		31.815 25.643 26.718 1.00 35.24
ATOM		31.107 25.754 25.406 1.00 34.57
MOTA	1510 C GLN A 203	30.218 26.586 25.256 1.00 34.62
MOTA	1511 O GLN A 203	31.317 24.446 27.514 1.00 35.59
ATOM	1512 CB GLN A 203	
ATOM	1513 CG GLN A 203	• • • • • • • • • • • • • • • • • • •
MOTA	1514 CD GLN A 203	
MOTA	1515 OE1 GLN A 203	
MOTA	1516 NE2 GLN A 203	
ATOM	1517 N GLN A 204	31.524 24.939 24.443 1.00 33.68
MOTA		30.873 24.899 23.165 1.00 32.97
MOTA	1519 C GLN A 204	29.714 23.959 23.373 1.00 32.67
MOTA	1520 O GLN A 204	29.838 22.982 24.082 1.00 32.33
MOTA	1521 CB GLN A 204	31.793 24.352 22.093 1.00 32.85
MOTA	1522 CG GLN A 204	33.042 25.165 21.819 1.00 32.50
MOTA	1523 CD GLN A 204	32.786 26.454 21.057 1.00 30.59
ATOM		
ATOM	1525 NE2 GLN A 204	33.843 27.132 20.664 1.00 29.18
MOTA	1526 N ASN A 205	28.583 24.247 22.755 1.00 32.81
ATOM		27.393 23.446 22.980 1.00 32.85
ATOM		26.594 23.059 21.733 1.00 32.80
ATOM		26.147 23.921 20.968 1.00 32.72
ATOM		26.484 24.246 23.919 1.00 32.83
ATOM		25.178 23.566 24.205 1.00 32.43
ATOM		24.914 22.465 23.732 1.00 32.78
ATOM		24.339 24.228 24.993 1.00 31.52
ATOM		26.427 21.763 21.515 1.00 32.36
ATOM		25.454 21.326 20.541 1.00 32.02
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MOTA	1536	_	מנות	7	206	24 167	00 077	01 201	1 00 01 50	~
			PHE .			24.167		21.301	1.00 31.59	C
ATOM	1537		PHE .			24.144		22.096	1.00 31.13	0
MOTA	1538	CB	PHE .	Α	206	25.972	20.159	19.754	1.00 32.17	C
MOTA	1539	CG	PHE .	Α	206	26.844	20.554	18.639	1.00 32.42	С
MOTA	1540	CD1	PHE .	Α	206	26.364	21.354	17.630	1.00 33.16	С
ATOM	1541	CD2	PHE	Α	206	28.149		18.600	1.00 33.19	С
ATOM	1542		PHE			27.174		16.600	1.00 33.34	Č
ATOM	1543		PHE			28.963		17.580	1.00 33.34	Ċ
MOTA	1544	CZ	PHE			28.485		16.574	1.00 33.50	С
MOTA	1545	N	PHE			23.104		21.012	1.00 31.65	. И
MOTA	1546	CA	PHE			21.829		21.726	1.00 31.71	С
ATOM	1547	C	PHE			20.822		20.924	1.00 31.35	C
MOTA	1548	0	PHE	Α	207	20.289	21.292	19.930	1.00 30.81	0
ATOM	1549	CB	PHE	Α	207	21.391	23.148	21.883	1.00 31.56	С
ATOM	1550	CG	PHE			20.118		22.683	1.00 31.43	Ċ
ATOM	1551		PHE			18.926		22.036	1.00 32.30	č
ATOM	1552		PHE			20.150		24.058	1.00 32.30	Č
ATOM	1553		PHE			17.781				
								22.748	1.00 32.37	C
ATOM	1554		PHE			19.006		24.776	1.00 31.14	С
ATOM	1555	CZ	PHE			17.828		24.122	1.00 32.27	С
MOTA	1556	Ν.	ALA			20.554		21.368	1.00 31.31	N
ATOM .	1557	CA	ALA			19.685	18.672	20.611	1.00 31.33	С
MOTA	1558	C	ALA	Α	208	18.264		21.138	1.00 31.59	С
MOTA	1559	0	ALA	Α	208	18.016	17.860	22.133	1.00 31.13	0
MOTA	1560	CB	ALA	Α	208	20.293	3 17.334	20.537	1.00 30.98	С
ATOM	1561	N	GLN	A	209	17.340	-	20.409	1.00 32.00	N
MOTA	1562	CA			209	15.939		20.751	1.00 32.37	С
ATOM	1563	С	GLN			15.288		20.358	1.00 32.76	Č
ATOM	1564	0			209	15.492		19.247	1.00 32.19	ō
ATOM	1565	СВ			209	15.24		20.031	1.00 32.15	c
ATOM	1566	CG			209	13.80		20.470	1.00 32.33	c
ATOM	1567	CD			209					
ATOM	1568					13.689		21.925	1.00 32.27	C
		OE1			209	14.69		22.587	1.00 31.73	0
MOTA	1569	NE2			209	12.45		22.436	1.00 32.63	N
MOTA	1570	N			210	14.46		21.272	1.00 33.20	N
MOTA	1571	CA			210	13.90		21.165	1.00 33.55	С
ATOM	1572	C			210	12.39		21.195	1.00 33.37	С
MOTA	1573	0			210	11.78		20.369	1.00 33.25	0
MOTA	1574	CB			210	14.45	6 15.210	22.302	1.00 33.79	С
MOTA	1575	CG1	ILE	Α	210	15.90	0 14.837	21.980	1.00 34.71	. С
MOTA	1576	CG2	ILE	Α	210	13.60	4 13.982	22.528	1.00 33.99	С
MOTA	1577	CD1	ILE	Α	210	16.67	9 14.375	23.191	1.00 35.48	. С
MOTA	1578	N			211	11.80			1.00 33.27	N
MOTA	1579	CA			211	10.36			1.00 33.48	C
MOTA	1580	C			211	9.96			1.00 33.68	C
MOTA	1581	Ö			211	10.54			1.00 34.10	Õ
ATOM	1582	СВ			211	9.86			1.00 33.57	Č
ATOM	1583	CG			211	8.35				
ATOM	1584				211				1.00 34.06	С
		CD							1.00 34.79	C
ATOM	1585	CE			211	6.63			1.00 35.65	C
ATOM	1586	NZ			211	5.87			1.00 36.67	N
MOTA	1587	N			212	8.93			1.00 34.06	N
MOTA	1588	CA			212	8.46			1.00 34.09	C
MOTA	1589	С			212	9.27			1.00 34.27	C
MOTA	1590	0			212	10.15			1.00 34.27	0
MOTA	1591	N	TYR	A	213	8.95	5 22.237	21.523	1.00 34.23	N
ATOM	1592	CA	TYR	A	213	9.64			1.00 34.12	С
MOTA	1593	С			213	10.21			1.00 33.81	C
ATOM	1594	O			213	9.60			1.00 33.09	ō
MOTA	1595	СВ			213					Č
MOTA	1596	CG			213	8.25			1.00 35.40	č
			_ ~~							C

ATOM	1597	CD1	TYR A 21	3	7.228	22.163	18.955	1.00 3	6.80		С
MOTA	1598		TYR A 21:		8.929	23.122	17.586	1.00 3	6.00		С
ATOM	1599	CE1	TYR A 21	3	6.873	21.323	17.944	1.00 3			С
MOTA	1600	CE2	TYR A 21	3	8.579	22.292	16.567	1.00 3			C
ATOM	1601	CZ	TYR A 21		7.560	21.390	16.743	1.00 3			C
MOTA	1602	OH	TYR A 21		7.242	20.568	15.688	1.00 4			0
MOTA	1603	N	LYS A 21		11.410	24.804	21.517	1.00 3			N
MOTA	1604	CA	LYS A 21		12.046	25.809	22.359	1.00 3		•	C
MOTA	1605	С	LYS A 21		12.479	27.033	21.551	1.00 3		_	C
MOTA	1606	0	LYS A 21		13.173	26.918		1.00		•	C .
MOTA	1607	CB	LYS A 21		13.237	25.208	23.101	1.00 3			C
MOTA	1608	CG	LYS A 21		12.881	24.443	24.364	1.00			C
ATOM	1609	CD	LYS A 21		14.126	23.861	24.973	1.00			c
MOTA	1610	CE	LYS A 21		14.001	23.615	26.458 27.130	1.00			N
ATOM	1611	NZ	LYS A 21		15.346 12.043	23.419 28.205	21.986	1.00			N
ATOM	1612	N	ARG A 21 ARG A 21		12.479	29.427	21.339	1.00			Ċ
ATOM	1613	CA	ARG A 21		13.816	29.427	21.944	1.00			C
ATOM	1614 1615	С 0	ARG A 21		13.946	29.923	23.146				ō
ATOM	1616	СВ	ARG A 21		11.482	30.552	21.558	1.00			C
ATOM ATOM	1617	CG	ARG A 21		11.865	31.844	20.885	1.00			С
ATOM	1618	CD	ARG A 21		11.287	33.028	21.593	1.00			С
ATOM	1619	NE	ARG A 23		11.381	34.255	20.823	1.00			N
ATOM	1620	CZ	ARG A 2		10.688	35.346	21.103	1.00			С
ATOM	1621		ARG A 2		9.860	35.371	22.144		34.68		N
ATOM	1622		ARG A 2		10.829	36.415	20.344	1.00	35.16		N
ATOM	1623	N	CYS A 2		14.810	29.962	21.092	1.00	33.76		N
MOTA	1624	CA	CYS A 2		16.152	30.238	21.542	1.00	33.91		С
ATOM	1625	С	CYS A 2		16.555	31.613	21.068	1.00	34.31		С
ATOM	1626	0	CYS A 2	16	16.534	31.885	19.872	1.00	34.69		0
MOTA	1627	CB	CYS A 2	16	17.099	29.189	20.968		33.84	_	С
MOTA	1628	SG	CYS A 2	16	16.655	27.490	21.397		32.85		S
MOTA	1629	N	ILE A 2		16.886	32.494	22.004		34.57		N
MOTA	1630		ILE A 2		17.335	33.830	21.648		34.82		C
MOTA	1631	С	ILE A 2		18.785	33.999	22.046		34.50		C
MOTA	1632		ILE A 2		19.136		23.213		34.30	•	O C
MOTA	1633		ILE A 2		16.475	34.890	22.324		35.07		C
MOTA	1634				15.003		22.001		35.20		c
ATOM	1635		2 ILE A 2		16.881		21.844 22.722		35.38 36.16		C
ATOM	1636		L ILE A 2		14.086 19.620	35.585 34.315	21.060		34.32		N
MOTA	1637		LEU A 2		21.052		21.277		34.44		C
MOTA	1638 1639		LEU A 2		21.565		21.017		34.27		Č
MOTA MOTA	1640		LEU A 2		21.074		20.148		34.59		0
MOTA	1641		LEU A 2		21.818				34.57		C
MOTA	1642				21.953				34.62		С
ATOM	1643		1 LEU A 2		20.614				34.96		С
MOTA	1644		2 LEU A 2		22.638				35.31		С
ATOM	1645		PHE A		22.594				33.79		N
MOTA	1646				23.258		21.632	1.00	33.40	•	С
· ATOM	1647		PHE A		24.730	37.155	21.617	1.00	33.29		С
ATOM	1648	3 0	PHE A	219	25.222				33.45		0
MOTA	1649				22.964				33.37		C
MOTA	1650				21.509				33.91		C
MOTA	165		1 PHE A		20.852				33.73		C
ATOM	.165		2 PHE A		20.794				33.70		C
MOTA	165		1 PHE A		19.512				33.52		C
MOTA	165		2 PHE A		19.460				33.47		C
MOTA	165				18.818				33.23		C
MOTA	165		PRO A		25.438				33.46		И С
MOTA	165	7 C.	A PRO A	220	26.888	37.496	20.536	3 I.UC	33.50		C

ATOM	1658		PRO A 2		27.675	38.131	21.699	1.00 3			С
MOTA	1659		PRO A		27.185	39.049	22.363	1.00 3			0
MOTA	1660		PRO A		27.246	38.169	19.211		3.51		C
MOTA	1661	CG	PRO A		25.977	38.683	18.629		3.41		C
ATOM	1662	CD	PRO A		24.869	38.462	19.544	1.00 3			C
ATOM	1663	N	PRO A		28.886	37.627	21.942	1.00 3			N
ATOM	1664	CA	PRO A		29.731	38.102	23.044		3.30		C
ATOM	1665	C	PRO A		29.966	39.581	23.081		3.55		C
ATOM	1666	0	PRO A		30.043	40.151	24.147		3.66		0
ATOM	1667 1668	CB CG	PRO A		31.033 30.589	37.375 36.128	22.799 22.147	1.00 3			C
ATOM ATOM	1669	CD	PRO A		29.523	36.522	21.207		32.91		C
ATOM	1670	И	ASP A		30.009	40.217	21.933	1.00 3			N
ATOM	1671	CA	ASP A		30.277	41.628	21.904	1.00 3			C
ATOM	1672	C	ASP A		29.073	42.419	22.382	1.00 3			. c
ATOM	1673	Ö	ASP A		29.048	43.634	22.241		34.68		ő
ATOM	1674	СВ	ASP A		30.679	42.055	20.502		34.79		Č
ATOM ·	1675	CG	ASP A		29.508	42.228	19.608	1.00 3			č
ATOM	1676		ASP ·A		28.387	41.897	20.028	1.00 3			ō
ATOM	1677		ASP A		29.601	42.692	18.462	1.00 4			Ö
MOTA	1678	N	GLN A		28.062	41.760	22.930		34.48		N
ATOM	1679	CA	GLN A		26.965	42.532	23.497	1.00 3		t	C
ATOM	1680	С	GLN A		27.031	42.541	25.011	1.00 3			С
ATOM	1681	0	GLN A		26.077	42.878	25.686	1.00 3	34.70		0
MOTA	1682	СВ	GLN A		25.595	42.133	22.940	1.00	34.87		С
MOTA	1683	CG	GLN A		25.364	42.825	21.599	1.00	36.55		С
ATOM	1684	CD	GLN A	223	23.990	42.635	21.020	1.00	39.56		С
MOTA	1685	OE1	GLN A	223	22.986	42.824	21.701	1.00	42.40		0
MOTA	1686	NE2	GLN A	223	23.936	42.294	19.742	1.00	41.89		N
MOTA	1687	N	PHE A	224	28.198	42.219	25.534	1.00			N
MOTA	1688	CA	PHE A	224	28.437	42.270	26.965	1.00			С
ATOM	1689	С	PHE A		27.941	43.571	27.570	1.00			С
MOTA	1690	0	PHE A		27.310	43.549	28.622	1.00			0
MOTA	1691	CB	PHE A		29.932	42.159	27.224	1.00			C
MOTA	1692	CG	PHE A		30.305	42.027	28.661		32.69		C
MOTA	1693		PHE A		30.429	43.137	29.476	1.00		•	C
MOTA	1694		PHE A		30.609	40.790	29.191	1.00			C
MOTA	1695		PHE A		30.821	43.003	30.817	1.00			C
MOTA	1696		PHE A		30.993	40.661	30.498		31.29		C
ATOM	1697	CZ	PHE A		31.098	41.775	31.316		30.73		C
ATOM	1698	N O.	GLU A		28.235	44.706	26.930		35.46		N
MOTA	1699	CA.	GLU A		27.852	45.994	27.492 27.608		35.85		C
MOTA	1700	C	GLU A		26.362	46.133 46.955	28.386		35.42 35.16		0
MOTA MOTA	1701 1702	O CB	GLU A GLU A		25.873 28.401	40.933	26.688		36.59		c
MOTA	1702	CG	GLU A		29.892	47.377	26.917		39.78		č
MOTA	1704	CD	GLU A		30.357	48.822	27.125		43,65		c
ATOM	1705		GLU A		29.937	49.524	28.099		44.64		Ö
ATOM	1706		GLU A		31.224	49.234	26.319		47.74		Ö
. ATOM	1707	N	CYS A		25.633	45.329	26.851		35.07		N
ATOM	1708	CA	CYS A		24.192		26.842		34.93		C
ATOM	1709	C	CYS A		23.473	44.498	27.770		34.91		C
ATOM	1710	Ö	CYS A		22.266		28.019		34.86		Ō
ATOM	1711	СВ	CYS A		23.681				34.80		C
ATOM	1712	SG	CYS A		24.135		24.291		34.76		s
MOTA	1713	N	LEU A		24.191		28.296		34.47		N
ATOM	1714	CA	LEU A		23.509				34.57		C
MOTA	. 1715		LEU A		23.815				34.08		С
MOTA	1716	0	LEU A		23.122				33.57		0
MOTA	1717	CB	LEU A		23.739			1.00	34.97		C
MOTA	1718	CG	LEU A	227	22.883	41.127	27.047	1.00	36.04		С

	1710 003	TEIT 7 227	23.454	40.177 2	26.043	1.00 37.99	
ATOM		LEU A 227	21.474			1.00 36.66	
MOTA		LEU A 227				1.00 34.23	
MOTA	1721 N	TYR A 228	24.866			1.00 34.23	
MOTA	1722 CA	TYR A 228	25.172				
MOTA	1723 C	TYR A 228	25.163			1.00 33.81	
MOTA	1724 0	TYR A 228	24.294			1.00 33.87	
MOTA	1725 CB	TYR A 228	24.183			1.00 33.73	
ATOM	1726 CG	TYR A 228	24.153			1.00 33.50	
ATOM	1727 CD	1 TYR A 228	24.947		32.568	1.00 33.63	
ATOM		2 TYR A 228	23.312	45.853	31.086	1.00 35.03	
ATOM	1729 CE		24.903	47.932	31.924	1.00 .34.25	
ATOM	1730 CE		23.268		30.419	1.00 35.62	
	1731 CZ		24.068	48.106	30.848	1.00 35.60	
ATOM		_	24.027	49.324	30.203	1.00 36.79	
MOTA	1732 OH	PRO A 229	26.170	41.263	33.027	1.00 33.75	
MOTA	1733 N		26.255	40.032	33.791	1.00 33.73	
MOTA	1734 CA			40.313	35.231	1.00 33.32	
MOTA	1735 C	PRO A 229	26.538			1.00 33.73	
MOTA	1736 0	PRO A 229	27.228	41.263	35.530	1.00 33.73	
MOTA	1737 CB		27.449	39.319	33.169		
MOTA	1738 CG		28.264	40.366		1.00 33.66	
MOTA	1739 CD		27.334	41.457	32.156	1.00 34.15	
MOTA	1740 N	TYR A 230	25.992	39.509	36.122	1.00 32.95	
ATOM	1741 CA		26.330	39.654	37.510	1.00 32.64	
ATOM	1742 C		27.836	39.534	37.651	1.00 32.59	
MOTA	1743 0		28.536	39.020	36.793	1.00 32.76	
ATOM	1744 CE		25.713	38.547	38.351	1.00 32.25	
ATOM	1745 C		24.237	38.640	38.573	1.00 31.53	
ATOM		D1 TYR A 230	23.346	38.125	37.641	1.00 31.07	
		D2 TYR A 230	23.727	39.192	39.748	1.00 29.93	
MOTA		E1 TYR A 230	21.996	38.185	37.859	1.00 31.19	
MOTA		E2 TYR A 230	22.395			1.00 28.83	
ATOM			21.523		39.040	1.00 31.04	
MOTA	1750 C				39.272	1.00 32.40	
MOTA	1751 0		20.165			1.00 32.40	
MOTA	1752 N		28.328			1.00 32.75	
MOTA		A PRO A 231	29.725			1.00 32.73	
MOTA	1754 C		30.159				•
MOTA	1755 0		29.434			1.00 32.86	
MOTA	1756 C	B PRO A 231	29.768		40.533	1.00 32.82	
MOTA	1757 C	G PRO A 231	28.625		40.605		
ATOM	1758 C	D PRO A 231	27.576		. 39.751		
ATOM	1759 N	VAL A 232	31.387				
ATOM		CA VAL A 232	31.938	36.825	38.680		
ATOM	1761	VAL A 232	31.776	36.022			
ATOM		VAL A 232	31.546	34.826	39.906		
ATOM		CB VAL A 232	33.422	36.918	38.332		
ATOM		CG1 VAL A 232	34.13		38.721	1.00 31.82	
ATOM		CG2 VAL A 232	33.603		36.851	1.00 31.85	
		N HIS A 233	31.91				
ATOM		CA HIS A 233	31.81				
ATOM	_		30.38				
ATOM			30.13				
MOTA	- '	O HIS A 233					
ATOM		CB HIS A 233	32.66				
MOTA		CG HIS A 233	34.13				
ATOM		ND1 HIS A 233.	34.78				
ATOM		CD2 HIS A 233	35.08				
ATOM		CE1 HIS A 233	36.07				
ATOM	1775	NE2 HIS A 233	36.27				
ATOM	1776	N HIS A 234	29.42				
ATOM		CA HIS A 234	28.03				
ATOM		C HIS A 234	27.50				
OTA		O HIS A 234	27.93	2 34.325	41.06	8 1.00 33.26	

ATOM	1780	CB	HIS A 234	27.221	37.276	42.024	1.00 33.15	C
MOTA	1781		HIS A 234		37.383	42.531	1.00 32.96	С
MOTA	1782		HIS A 234		36.704	41.951	1.00 32.53	. N
MOTA	1783		HIS A 234		38.191	43.471	1.00 32.12	С
ATOM	1784		HIS A 234		37.056	42.540	1.00 32.45	С
ATOM	1785		HIS A 234		37.953	43.470	1.00 32.09	N
ATOM	1786	N	PRO A 235		34.263	42.827	1.00 33.15	N
ATOM	1787	CA	PRO A 235		32.996	42.410	1.00 32.79	C
ATOM ATOM	1788	C	PRO A 23		33.045	41.026	1.00 32.62	C
ATOM	1789 1790	O CB	PRO A 23		31.990	40.440	1.00 32.65 1.00 33.00	0
ATOM	1791	CG	PRO A 23.		32.773 33.500	43.450 44.672	1.00 33.00	C C
ATOM	1792	CD	PRO A 23		34.725	44.128	1.00 32.79	c
ATOM	1793	N	CYS A 23		34.725	40.493	1.00 33.00	N
ATOM	1794	CA	CYS A 23		34.286	39.185	1.00 32.33	C
ATOM	1795	C	CYS A 23		34.640	38.139	1.00 32.34	Č
MOTA	1796	Ö	CYS A 23		35.034	37.018	1.00 32.23	ō
ATOM	1797	СВ	CYS A 23		35.192	39.206	1.00 32.02	Č
MOTA	1798	SG	CYS A 23		34.545	40.326	1.00 32.09	S
ATOM	1799	N	ASP A 23		34.456	38.511	1.00 32.71	N
MOTA	1800	CA	ASP A 23		34.609	37.576	1.00 33.21	С
MOTA	1801	С	ASP A 23		34.022	36.211	1.00 33.63	С
MOTA	1802	0	ASP A 23	7 27.042	32.911	36.095	1.00 33.33	0
MOTA	1803	CB	ASP A 23	7 29.139	33.964	38.132	1.00 33.01	С
MOTA	1804	CG	ASP A 23		33.981	37.151	1.00 33.76	С
MOTA	1805		ASP A 23		34.874	36.279	1.00 34.52	0
MOTA	1806	OD2	ASP A 23		33.135	37.181	1.00 36.09	0
MOTA	1807	N	ARG A 23		34.821	35.180	1.00 34.68	N
MOTA	1808	CA	ARG A 23		34.451	33.810	1.00 35.15	С
MOTA	1809	С	ARG A 23		34.690	33.375	1.00 34.98	С
MOTA	1810	0	ARG A 23		34.543	32.197	1.00 34.26	0
MOTA	1811	CB	ARG A 23		33.020	33.561	1.00 35.64	C
MOTA	1812	CG	ARG A 23		32.847	33.620	1.00 36.86	. C
MOTA	1813	CD	ARG A 23		31.474	33.268	1.00 38.59	C
MOTA MOTA	1814 1815	NE	ARG A 23		30.549 29.755	34.338	1.00 41.64	N
ATOM	1816	CZ	ARG A 23			34.286	1.00 43.17	· C
ATOM	1817		ARG A 23		29.802 28.923	33.218 35.291	1.00 44.38	N N
ATOM	1818	Nnz	GLN A 23		35.044	34.303	1.00 42.18 1.00 35.13	N
ATOM	1819	CA	GLN A 23		35.360	33.920	1.00 35.13	C
ATOM	1820	C	GLN A 23		36.872	33.825	1.00 33.15	C
ATOM	1821	Ö	GLN A 23			34.539	1.00 34.65	Ö
ATOM	1822	СВ	GLN A 23			34.921	1.00 35.27	c
ATOM	1823	CG	GLN A 23			35.566	1.00 37.30	c
MOTA	1824	CD	GLN A 23			34.552	1.00 41.59	Ċ
MOTA	1825		GLN A 2			33.726	1.00 45.42	0
ATOM	1826	NE	2 GLN A 2			34.609	1.00 42.92	N
MOTA	1827	N	SER A 2			32.930	1.00 33.99	N
MOTA	1828	CA	SER A 2	0 22.455	38.785	32.802	1.00 33.14	С
MOTA	1829	С	SER A 2	0 21.613	39.254	33.957	1.00 32.53	С
MOTA	1830	0	SER A 2		38.528	34.446	1.00 31.77	0
MOTA	1831	CB	SER A 2			31.542	1.00 33.15	C
MOTA	1832		SER A 2			31.668	1.00 33.28	0
ATOM	1833		GLN A 2			34.371	1.00 32.52	N
ATOM	1834					35.476	1.00 32.54	C
ATOM	1835		GLN A 2			35.001	1.00 32.44	С
ATOM	1836		GLN A 2			35.804	1.00 32.16	.0
ATOM	1837		GLN A 2				1.00 32.36	C
MOTA MOTA	1838 1839					36.917	1.00 32.74	Ö
MOTA	1840		GLN A 2 1 GLN A 2			37.450	1.00 33.65	C
AION	T040	OE.	T GDM W Z	23.353	43.442	38.428	1.00 34.26	0

MOTA	1841 NE2 GLN A 241	24.858 43.182 36.794 1.00 35.62	N
MOTA	1842 N VAL A 242	19.513 41.708 33.705 1.00 32.07	N
ATOM	1843 CA VAL A 242	18.357 42.412 33.255 1.00 32.29	С
		17.162 41.521 33.265 1.00 31.93	. c ·
MOTA		17.221 40.442 32.734 1.00 32.93	0
MOTA	1845 O VAL A 242		Č
MOTA	1846 CB VAL A 242		C
MOTA	1847 CG1 VAL A 242	17.252 43.532 31.320 1.00 32.50	C
MOTA	1848 CG2 VAL A 242	19.717 43.714 31.655 1.00 33.06	С
ATOM	1849 N ASP A 243	16.067 41.977 33.838 1.00 31.76	N
ATOM	1850 CA ASP A 243	14.812 41.271 33.714 1.00 31.73	С
MOTA	1851 C ASP A 243	14.177 41.559 32.346 1.00 31.87	С
	1852 O ASP A 243	13.536 42.595 32.150 1.00 31.46	
ATOM		13.861 41.689 34.830 1.00 31.61	
ATOM	1853 CB ASP A 243		•
ATOM	1854 CG ASP A 243	70	
MOTA	1855 OD1 ASP A 243		
MOTA	1856 OD2 ASP A 243	11.654 41.103 35.635 1.00 33.90	
ATOM	1857 N PHE A 244	14.326 40.623 31.410 1.00 32.16	
ATOM	1858 CA PHE A 244	13.746 40.787 30.075 1.00 32.29	
MOTA	1859 C PHE A 244	12.252 41.087 30.092 1.00 32.74	
ATOM	1860 O PHE A 244	11.741 41.694 29.162 1.00 32.51	. 0
MOTA	1861 CB PHE A 244	13.963 39.559 29.220 1.00 31.99	C
		15.327 39.446 28.650 1.00 31.29	
MOTA			
MOTA	1863 CD1 PHE A 244		
MOTA	1864 CD2 PHE A 244		
ATOM	1865 CE1 PHE A 244	17.684 39.733 28.815 1.00 31.37	
ATOM	1866 CE2 PHE A 244	16.742 38.709 26.888 1.00 31.39	
AŤOM	1867 CZ PHE A 244	17.839 39.141 27.584 1.00 31.7	
MOTA	1868 N ASP A 245	11.547 40.646 31.124 1.00 33.52	·
MOTA	1869 CA ASP A 245	10.130 40.946 31.214 1.00 34.3	3 C
MOTA	1870 C ASP A 245	9.831 42.375 31.606 1.00 34.53	2 C
MOTA	1871 O ASP A 245	8.789 42.902 31.251 1.00 34.4	0
MOTA	1872 CB ASP A 245	9.448 40.015 32.188 1.00 34.5	9 C
MOTA	1873 CG ASP A 245	9.361 38.639 31.658 1.00 35.4	7 C
MOTA	1874 OD1 ASP A 245	9.282 38.519 30.420 1.00 36.4	0 0
ATOM	1875 OD2 ASP A 245	9.384 37.624 32.383 1.00 37.6	
	1876 N ASN A 246	10.737 43.000 32.339 1.00 35.0	
MOTA		10.531 44.364 32.776 1.00 35.3	
MOTA	= - ·	11.873 45.003 32.896 1.00 34.9	
MOTA	1878 C ASN A 246		
MOTA	1879 O ASN A 246		
MOTA	1880 CB ASN A 246		
MOTA	1881 CG ASN A 246		
ATOM	1882 · OD1 ASN A 246	9.241 46.691 33.682 1.00 38.9	
MOTA	1883 ND2 ASN A 246	9.186 46.006 35.836 1.00 38.9	
· ATOM	1884 N PRO A 247	12.468 45.357 31.766 1.00 34.8	
ATOM	1885 CA PRO A 247	13.816 45.931 31.766 1.00 34.8	
MOTA		13.868 47.295 32.407 1.00 34.8	
ATOM		13.038 48.159 32.127 1.00 34.8	
ATOM		14.184 46.046 30.288 1.00 34.7	
ATOM		13.028 45.475 29.507 1.00 34.9	95 C
ATOM		11.892 45.241 30.419 1.00 34.	75 C
		14.861 47.448 33.270 1.00 34.0	
MOTA		15.112 48.654 34.003 1.00 34.	
ATOM		16.205 49.419 33.294 1.00 34.5	
ATOM		17.395 49.240 33.568 1.00 34.	
ATOM			
ATOM			
ATOM			
ATOM		15.958 50.583 35.902 1.00 34.	
ATOM		15.574 49.259 37.550 1.00 36.	
ATOM		15.793 50.302 32.399 1.00 35.	
ATON		16.743 51.063 31.615 1.00 35.	
OTA	1 1901 C TYR A 249	17.578 52.071 32.400 1.00 35.	48 C

ATOM	1902	0	TYR	Α	249		18.570	52.567	31.880	1.00	35.44	0
ATOM	1903	CB	TYR				16.021	51.741	30.465		35.05	C
ATOM	1904	CG	TYR				15.304	50.761	29.586		34.41	Č
MOTA	1905	CD1	TYR				15.977	49.718	28.971		34.17	C
MOTA	1906		TYR				13.955	50.865	29.383		34.14	
MOTA.	1907	CE1	TYR				15.312	48.828	28.172		33.95	C
MOTA	1908	CE2	TYR				13.287	49.983	28.595		33.71	c
MOTA	1909	CZ	TYR				13.954	48.974	27.989		34.19	
MOTA	1910	ОН	TYR				13.232	48.113	27.194			C
ATOM	1911	N	GLU				17.207	52.393	33.631		35.64	0
ATOM	1912	CA	GLU				18.072	53.273	34.399		35.82	N
ATOM	1913	C	GLU				19.331	52.562	34.834		36.69	С
	. 1914	Ö	GLU				20.424	53.102	34.715		36.69 36.84	C
ATOM	1915.	СВ	GLU				17.369	53.836	35.607			0
ATOM	1916	CG	GLU				16.173	54.653	35.195		37.10	C
ATOM	1917	CD			250		15.559	55.362	36.359		39.48 42.67	C
ATOM	1918		GLU				16.128	55.258	37.469			C
ATOM	1919	OE2					14.529	56.030			45.95	0
MOTA	1920	N			251		19.202	51.344	36.160		44.93	0
ATOM	1921	CA			251		20.389	50.666	35.332		36.55	N
ATOM	1922	C	ARG				21.124	50.162	35.773 34.584		36.36	C
ATOM	1923	Õ			251		22.347	50.102			35.91	C
ATOM	1924	СВ			251				34.588		36.89	0
ATOM	1925	CG			251		20.062 19.329	49.495	36.697		36.66	C
ATOM	1926	CD			251		18.848	49.936	37.981		38.10	C
ATOM	1927	NE			251		19.969	48.824	38.916		39.00	C
ATOM	1928	CZ			251		19.895	48.005	39.371		40.55	N
ATOM	1929		ARG				18.742	46.712	39.648		41.33	C
ATOM	1930		ARG					46.068	39.542		42.58	N
ATOM	1931	N			252		20.978	46.058	40.025		41.49	N
ATOM	1932	CA			252		20.388	49.807	33.545		35.06	N
MOTA	1933	C			252		20.988	49.065	32.455		34.37	C
ATOM	1934	0			252		20.653	49.675	31.138		33.82	C
ATOM	1935	CB					20.048	49.042	30.278		33.57	0
ATOM	1936	CG			252 252		20.429	47.662	32.458		34.19	C
ATOM	1937	CD1			252		20.404	47.019	33.803		33.98	. C
ATOM	1938		PHE				21.559	46.855	34.532		33.98	С
ATOM	1939		PHE				19.220	46.560	34.337		32.84	C
ATOM	1940	CE2			252		21.519	46.238	35.760		33.51	C
ATOM	1941	CZ			252		19.189	45.953	35.560		32.14	C
ATOM	1942	N			253		20.327	45.789	36.269		31.96	C
ATOM	1943	CA			253		21.087	50.903	30.959		33.27	N
ATOM	1944	C					20.677	51.675	29.795		32.92	C
	. 1945	Ö			253 253		21.008	50.995	28.470		32.86	C
ATOM	1946	СВ			253		20.215	51.136	27.541		32.58	0
ATOM	1947	CG				•	21.464	52.957	29.962		32.58	С
ATOM	1948	CD			253		22.584	52.562	30.808		32.44	C
ATOM	1949				253		22.038	51.640	31.802		32.67	C
MOTA	1950	N			254		22.108	50.253	28.359		32.60	N
ATOM	1951	CA			254		22.419	49.726	27.037		32.87	С
ATOM		С			254		21.564	48.569	26.615		32.59	С
MOTA	1952	0			254		21.671	48.088	25.503		32.69	0
	1953	CB			254		23.892	49.414	26.852		32.72	C
MOTA	1954	CG			254		24.710	50.665	26.745		33.92	C
MOTA	1955		ASN				25.428	51.022	27.672		37.05	0
ATOM	1956		ASN				24.569	51.380	25.626		34.86	N
ATOM	1957	N			255		20.690	48.124	27.491		32.37	N
MOTA	1958	CA			255		19.834	47.057	27.101		32.19	С
ATOM	1959	C.			255		18.932	47.578	26.006		32.36	С
ATOM	1960	0			255		18.267	46.819	25.326		32.64	0
ATOM	1961	CB			255		18.990	46.572	28.250		31.93	С
MOTA	1962	CG	PHE	A	255		18.249	45.354	27.918	1.00	31.43	C

											•
ATOM	1963	CD1 PI	HE A 25	55	18.919			1.00 33			C
ATOM	1964	CD2 PI	HE A 2	55	16.909	45.392	27.718	1.00 33			С
MOTA	1965	CE1 PI	HE A 2	55	18.239	43.035	27.367	1.00 3	4.05	•	С
ATOM			HE A 2		16.230	44.275	27.380	1.00 3	2.00		С
			HE A 2		16.890	43.088	27.203	1.00 3			С
ATOM					18.890	48.888	25.844	1.00 3			N
ATOM			LN A 2					1.00 3			N C
MOTA			LN A 2		18.078	49.456	24.794				C
MOTA	1970		LN A 2		18.776	49.342	23.455	1.00 3			
ATOM	1971	O G	LN A 2	56	18.260	49.815	22.470	1.00 3			0
ATOM	1972	CB G	LN A 2	56	17.777	50.924	25.061	1.00 3			C
ATOM	1973		LN A 2		16.775	51.169	26.144	1.00 3	2.39		C
ATOM	1974		LN A 2		16.823	52.594	26.645	1.00 3	2.91		С
ATOM	1975		LN A 2		15.830	53.303	26.588	1.00 3			0
	1976		LN A 2		17.982	53.021	27.125	1.00 3			N
ATOM					19.956	48.744	23.404	1.00 3			N
MOTA	1977		SN A 2					1.00 3			Ĉ
ATOM	1978		ASN A 2		20.634	48.617	22.126			•	Č
MOTA	1979		ASN A 2		20.828	47.159	21.763	1.00 3			
MOTA	1980	O	ASN A 2	257	21.406	46.841	20.721	1.00 3			0
ATOM	1981	CB F	ASN A 2	257	21.998	49.310	22.140	1.00 3			С
ATOM	1982	CG F	ASN A 2	257	21.928	50.750	22.595	1.00 3	31.31		С
ATOM	1983		ASN A 2		22.471	51.105	23.639	1.00 2	27.26		0
	1984		ASN A 2		21.283	51.595	21.797	1.00 2			N
ATOM					20.338	46.263	22.606	1.00			N
MOTA	1985		VAL A				22.370	1.00			Ċ
ATOM	1986		VAL A		20.565			1.00			Č
MOTA	1987		VAL A		19.832	44.361	21.130				Ö
MOTA	1988	0 '	VAL A	258	18.751		20.813	1.00			
MOTA	1989	CB '	VAL A	258	20.144		23.558	1.00			C
ATOM	1990	CG1	VAL A	258	18.632	43.851	23.604	1.00	35.73		· C
ATOM	1991	CG2	VAL A	258	20.780	42.662	23.428	1.00			С
ATOM	1992		VAL A		20.447		20.428	1.00	35.87		N
ATOM	1993		VAL A		19.853		19.230		36.40		С
	1994		VAL A		20.125		19.148		36.66		С
MOTA					21.282		19.102		36.47		0
ATOM	1995		VAL A						36.47	•	Č
ATOM	1996		VAL A		20.450		17.969				Č
MOTA	1997		VAL A		19.830		16.764		36.75		C
ATOM	1998		VAL A		20.212				36.66	•	
ATOM	1999	N	GLY A	260	19.066				37.15		N
MOTA	2000	CA	GLY A	260	19.215	39.096	19.067		37.50		С
ATOM	2001	С	GLY A	260	19.132	38.328	17.745		37.55		C
MOTA	2002		GLY A		18.716	38.839	16.704	1.00	37.45	•	0
MOTA	2003		TYR A		19.578			1.00	37.54		N
ATOM	2004		TYR A		19.466		. 16.744	1.00	37.52		. C
			TYR A		18.530				37.09		С
ATOM	2005				18.788				37.12		0
MOTA	2006		TYR A						37.79		Ċ
MOTA	2007		TYR A		20.79						
MOTA	2008		TYR A		21.83				39.43		C
ATOM	2009		TYR A		22.00				41.03		С
ATOM	2010	CD2	TYR A	261	22.64	8 . 37.125	16.662		41.07		С
MOTA	2011	. CE1	TYR A	261	22.93	7 37.193	3 13.940		41.71		C
ATOM	2012		TYR A		23.59			1.00	41.99		С
ATOM	2013		TYR A		23.72				42.45		С
ATOM	2014		TYR A		24.65				46.29		0
					17.43				36.56		N
MOTA			GLU A						35.87		Ċ
ATOM			GLU A		16.50				35.41		c
MOTA			GLU A		16.06						0
MOTA			GLU A		16.31				35.03		
MOTA			GLU A		15.32				35.67		C
ATOM	2020	CG	GLU A	262	14.08				35.22		C
MOTA		1 CD	GLU A	262	13.03				35.62		C
ATOM			GLU A	262	13.20	1 36.83	3 17.86	1.00	38.15		0
ATOM			GLU A		12.07	4 35.03	1 18.36	7 1.00	35.12		0

MOTA	2024	N	THR	Α	263	15.440	31.744	17.060	1.00 35.07	N
ATOM	2025	CA	THR	A	263	15.004	30.565	16.351	1.00 34.84	C
MOTA	2026	C	THR			14.138	29.670	17.224	1.00 34.38	Ċ
MOTA	2027	0	THR	Α	263	14.152	29.745	18.452	1.00 34.07	0
MOTA	2028	CB	THR	Α	263	16.235	29.767	15.847	1.00 34.75	Ċ
ATOM	2029	OG1	THR	Α	263	15.864	28.964	14.731	1.00 35.81	0
MOTA	2030	CG2	THR	A	263	16.693	28.745	16.837	1.00 34.59	C
MOTA	2031	N	VAL	A	264	13.368	28.820	16.573	1.00 34.02	N
MOTA	2032	CA	VAL	Α	264	12.597	27.854	17.306	1.00 33.95	C
MOTA	2033	С	VAL	Α	264	13.054	26.460	16.918	1.00 33.60	C
MOTA	2034	0	VAL	Α	264	12.957	26.065	15.762	1.00 33.27	0
ATOM	2035	CB	VAL			11.112	28.019	17.075	1.00 33.95	C
ATOM	2036	CG1	VAL	Α	264	10.393	26.788	17.568	1.00 34.24	C
MOTA	2037	CG2	VAL	Α	264	10.615	29.247	17.823	1.00 33.85	С
MOTA	2038	N	VAL	А	265	13.572	25.708	17.880	1.00 33.43	N
MOTA	2039	CA	VAL	Α	265	13.984	24.354	17.546	1.00 33.48	С
MOTA	2040	C	VAL	Α	265	12.949	23.321	17.907	1.00 32.85	C
MOTA	2041	0	VAL	A	265	12.234	23.441	18.884	1.00 32.91	0
MOTA	2042	CB	VAL	A	265	15.332	23.954	18.139	1.00 33.61	· C
MOTA	2043		VAL			16.408	24.721	17.432	1.00 34.56	С
ATOM	2044	CG2	VAL			15.381	24.153	19.636	1.00 33.15	С
ATOM	2045	N	GLY	Α	266	12.848	22.321	17.064	1.00 32.32	N
MOTA	2046	CA			266	11.938	21.240	17.331	1.00 32.27	С
ATOM	2047	С			266	12.634	1,9.905	17.310	1.00 31.78	С
ATOM.	2048	0			266	13.852	19.799	17.124	1.00 31.15	0
MOTA	2049	N ·	PRO	A	267	11.827	18.872	17.454	1.00 31.56	N
ATOM	2050	CA			267	12.343	17.516	17.547	1.00 31.40	· C
MOTA	2051	С			267	13.203	17.314	16.336	1.00 31.22	С
MOTA	2052	0			267	12.755	17.631	15.241	1.00 31.24	0
MOTA	2053	CB	PRO	Α	267	11.074	16.664	17.552	1.00 30.81	С
MOTA	2054	CG			267	10.048	17.568	18.087	1.00 31.26	C
MOTA	2055	CD			267	10.358	18.900	17.451	1.00 31.85	С
MOTA	2056	N			268	14.445	16.891	16.536	1.00 31.06	N
MOTA	2057	CA			268	15.334	16.620	15.426	1.00 31.07	С
MOTA	2058	С			268	16.337	17.703	15.112	1.00 31.31	С
MOTA	2059	0			268	17.352	17.425	14.493	1.00 31.12	0
MOTA	2060	N			269	16.061	18.939	15.517	1.00 31.87	N
MOTA	2061	CA			269	16.975	20.032	15.253	1.00 32.18	С
MOTA	2062	С			269	18.117	20.099	16.282	1.00 32.69	С
ATOM	2063	0			269	17.974	19.720	17.450	1.00 32.69	0
MOTA	2064	СВ			269	16.282	21.381	15.390	1.00 32.73	C
MOTA	2065	CG			269	15.094	21.583	14.478	1.00 32.07	С
ATOM	2066		ASP			15.023	21.039	13.367	1.00 33.96	0
ATOM	2067		ASP			14.191	22.368	14.806	1.00 30.81	0
MOTA	2068	N			270	19.234	20.667	15.854	1.00 32.97	N
MOTA	2069	CA			270	20.376	20.839	16.715	1.00 32.97	С
MOTA	2070	C			270	20.844	22.258	16.579	1.00 32.97	С
ATOM	2071	0			270	21.130	22.716	15.488	1.00 33.40	0
MOTA	2072	CB			270	21.485	19.896	16.323	1.00 32.94	С
ATOM	2073		VAL			22:755	20.207	17.066	1.00 33.16	С
ATOM	2074		VAL			21.069	18.519	16.646	1.00 33.14	С
MOTA	2075	N			271	20.883	22.965	17.692	1.00 32.91	N
ATOM	2076	CA			271	21.321	24.337	17.690	1.00 32.91	С
ATOM	2077	C			271	22.770	24.395	18.129	1.00 32.95	С
ATOM	2078	0			271	23.116	23.864	19.161	1.00 32.76	0
ATOM	2079	CB			271	20.468	25.159	18.656	1.00 32.64	С
MOTA	2080	CG			271	20.896	26.616	18.773	1.00 32.61	С
ATOM	2081		LEU			20.989	27.276	17.405	1.00 32.23	C
MOTA	2082		LEU			19.936	27.383	19.638	1.00 33.12	С
MOTA MOTA	2083	N			272	23.633	25.006	17.333	1.00 33.19	N
ALON	2084	CA	IIK	A	272	24.989	25.215	17.791	1.00 33.39	С

ATOM	2085	С	TYR A	272	25.004	26.517	18.554	1.00 3	3.40		С
MOTA	2086	0	TYR A	272	24.834	27.560	17.950	1.00 3			0
MOTA	2087	CB	TYR A	272	25.991	25.297	16.633	1.00 3			С
MOTA	2088	CG	TYR A	. 272	27.376	25.802	17.039	1.00 3		•	С
MOTA	2089	CD1	TYR A	. 272	28.005	25.340	18.179	1.00 3			C
ATOM	2090	CD2	TYR A	. 272	28.047	26.746	16.267	1.00 3			C
ATOM	2091	CE1	TYR A	. 272	29.265	25.805	18.544	1.00			С
ATOM	2092	CE2	TYR A		29.300	27.213	16.622	1.00			С
MOTA	2093	CZ	TYR A		29.906	26.737	17.759	1.00			C
MOTA	2094	OH	TYR A		31.146	27.216	18.113	1.00			0.
MOTA	2095	N	ILE F		25.178	26.438	19.872	1.00			N
MOTA	2096	CA	ILE A		25.350	27.609	20.734	1.00			C
MOTA	2097	C	ILE A		26.830	27.759	21.068	1.00			C
MOTA	2098	0	ILE A		27.332	27.113	21.998	1.00			0
MOTA	2099	CB	ILE A		24.595	27.436	22.032	1.00			C
ATOM	2100		ILE A		23.122	27.219	21.749	1.00			C
MOTA	2101	CG2	ILE A		24.779	28.654	22.896	1.00			C
MOTA	2102		ILE A		22.306	26.986	22.984		33.23		N
MOTA	2103	N		A 274	27.519	28.630	20.345		34.61		C
MOTA	2104	CA		A 274	28.965	28.780	20.485		34.92		C
MOTA	2105	С		A 274	29.348	29.378	21.803		35.17 35.16		0
ATOM	2106	0		A 274	28.639	30.252	22.300		35.10		c
ATOM	2107	CB		A 274	29.333	29.771	19.382		35.02		c
MOTA	2108	CG		A 274	28.113	29.929	18.551 19.388		34.69		č
ATOM	2109	CD		A 274	26.957	29.584	22.339		35.69		N
MOTA	2110	N		A 275	30.476	28.927 29.399	23.622		36.15	•	č
MOTA	2111	CA		A 275	30.982 30.981	30.917	23.754		36.09		č
ATOM	2112	C		A 275	31.316	31.635	22.805		36.23		Ö
ATOM .	2113	0		A 275	32.400	28.928	23.805	•	36.23		č
MOTA	2114	CB		A 275 A 275	32.400	28.928	25.229		38.02		Č
MOTA	2115	CG		A 275 A 275	34.361	28.108	25.442		42.07	,	S
MOTA	2116	SD CE		A 275	35.330	28.680	23.895		42.34		Č
ATOM ATOM	2117 2118	N		A 276	30.611	31.401	24.935		35.76		N
ATOM	2119	CA		A 276	30.574	32.833			35.62		С
ATOM	2120	C		A 276	29.339	33.513			35.32		C
ATOM	2121	Õ		A 276	29.048	34.653			35.15		0
ATOM .		СВ		A 276	31.921	33.510			35.75		С
ATOM	2123	CG		A 276	33.049	33.221		1.00	35.70		С
ATOM	2124			A 276	33.036			1.00	34.51		С
ATOM	2125	CD		A 276	34.103		25.521	1.00	35.30		C
ATOM	2126			A 276	34.013	33.549	27.997	1.00	34.63		С
ATOM	2127			À 276	35.100	32.085	26.446	1.00	35.01		C
MOTA	2128			A 276	35.055	32.685			35.73		C
ATOM	2129		TYR	A 276	36.051	32.433			34.27		0
MOTA	2130	N	TRP	A 277	28.573				35.19		N
ATOM	2131	CA		A 277	27.353				35.20		С
MOTA	2132	С		A 277.	26.245				35.16		C
MOTA	2133	0		A 277	25.947				35.08		0
MOTA	2134			A 277	26.806				35.27		C
MOTA	2135			A 277	27.538				34.70		C
MOTA	2136			A 277	28.858				35.11		C
ATOM	2137			A 277	27.020				35.27		C
MOTA	2138			A 277	29.213				35.58		N
MOTA	2139			A 277	28.094				34.89		C
MOTA	2140			A 277	25.75				35.56		C
MOTA	2141			A 277	27.94				32.83		C
ATOM	2142			A 277	25.612				34.41		C
MOTA	2143			A 277	26.70				33.11		N
MOTA	2144			A 278	25.59				35.11		C
ATOM	2145	5 CF	A TRE	A 278	24.50	1 34.612	2 25.388	. T.O(35.03		C

ATOM 2146 C TRP A 278										•	
ATOM 2148 CB TRP A 278		2146	С	TRP	A	278	23.334	33.859	24.838	1.00 35.14	
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM			0				23.068	33.939			Ō
ATOM 2150 CD1 TRP A 278							24.047		25.553		С
ATOM 2151 CD2 TRP A 278											С
ATOM 2153 (REI TRP A 278 26.713 38.336 26.518 1.00 36.09 ATOM 2153 (REZ TRP A 278 26.133 38.132 27.741 1.00 36.37 ATOM 2155 (REZ TRP A 278 26.463 38.637 28.976 1.00 37.12 ATOM 2155 (REZ TRP A 278 24.636 37.375 29.877 1.00 36.38 ATOM 2156 (REZ TRP A 278 24.636 37.375 29.877 1.00 36.37 ATOM 2157 (REZ TRP A 278 24.636 37.375 29.877 1.00 36.37 ATOM 2158 N HIS A 279 22.620 33.133 25.692 1.00 35.10 ATOM 2159 (REZ TRP A 278 22.620 33.133 25.692 1.00 35.10 ATOM 2159 (REZ TRP A 278 22.620 33.133 25.692 1.00 35.10 ATOM 2150 (REZ TRP A 279 22.600 33.133 25.692 1.00 35.10 ATOM 2160 (REZ TRP A 279 20.500 22.516 25.218 1.00 34.69 ATOM 2161 (REZ TRP A 279 20.500 32.555 26.231 1.00 34.69 ATOM 2162 (REZ HIS A 279 20.500 32.555 26.231 1.00 34.69 ATOM 2162 (REZ HIS A 279 21.640 30.23 2.348 27.414 1.00 34.75 ATOM 2162 (REZ HIS A 279 21.642 31.079 24.764 1.00 35.73 ATOM 2163 (REZ HIS A 279 22.010 29.283 26.609 1.00 38.10 ATOM 2165 (REZ HIS A 279 22.010 29.283 26.609 1.00 38.10 ATOM 2166 (REI HIS A 279 23.143 28.797 27.221 1.00 37.68 ATOM 2166 (REI HIS A 279 23.143 28.797 27.221 1.00 37.68 ATOM 2166 (REI HIS A 280 17.850 32.884 26.483 1.00 33.72 ATOM 2169 (REZ HIS A 280 17.850 32.884 26.483 1.00 33.72 ATOM 2169 (REZ HIS A 280 17.850 32.884 26.483 1.00 33.72 ATOM 2170 (RIS A 280 17.215 34.208 26.257 1.00 33.52 ATOM 2171 (RIS A 280 17.850 32.884 26.483 1.00 33.72 ATOM 2171 (RIS A 280 17.850 32.884 26.483 1.00 33.72 ATOM 2173 (REZ HIS A 280 15.733 34.247 26.486 1.00 33.57 ATOM 2170 (RIS A 280 17.850 32.884 26.483 1.00 33.72 ATOM 2171 (RIS A 280 15.733 34.204 26.557 1.00 33.567 ATOM 2173 (REZ HIS A 280 15.733 34.204 26.257 1.00 33.567 ATOM 2173 (REZ HIS A 280 15.733 34.204 26.257 1.00 33.567 ATOM 2173 (REZ HIS A 280 15.733 34.204 26.484 1.00 33.367 ATOM 2173 (REZ HIS A 280 15.733 34.204 26.384 1.00 33.92 ATOM 2174 (RIS A 280 15.573 34.204 25.344 1.00 33.367 ATOM 2176 (RIS A 280 13.545 34.078 25.344 1.00 33.367 ATOM 2185 (RIS A 280 13.545 34.078 25.344 1.00 33.367 ATOM 2180 (RIS A 280 13.545 34.078 25.344 1.00 33.367 ATOM 2180 (RIS A 280									•		C
ATOM 2154 CE2 TRP A 278											С
ATOM 2154 CB3 TRP A 278											N
ATOM 2155 C22 TRP A 278											С
ATOM 2156 C23 TRP A 278											С
ATOM 2157 CH2 TRP A 278											C
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ATOM 2166 CD2 HIS A 279	ATOM	2164	ND1								N
ATOM 2166 CE1 HIS A 279	ATOM	2165	CD2	HIS	Α	279					C
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ATOM 2169 CA HIS A 280			NE2					28.797	27.221	1.00 37.68	N
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3000 0000											0
AIOM 2200 CG LEO A 284 /.302 2/.255 21.596 1.00 35.52											С
	MION	2200	CG	TEU	A	404	1.302	27.255	21.596	1.00 35.52	С

ATOM	2207	CD1 I	LEU A	. 2	84	6.0	575	27.4	27	20.23	1 1	.00	36.06	5		С
ATOM		CD2 I				8.3	197	28.4	04	21.86	2 1	.00	36.37	7		С
MOTA	2209	N I	LEU A	. 2	85	4.	674	28.5	61	25.04	0 1	00	35.48	В		N
ATOM	2210	CA I	LEU A	. 2	85		481	28.6		25.83		00				С
ATOM	2211		LEU P				509	27.6		25.25		.00				С
MOTA	2212		LEU A				314	27.6		24.04		00				0
ATOM	2213	CB I	LEU A	1 2	85		876	30.0		25.74		1.00				С
MOTA	2214		LEU <i>I</i>				740	31.1		26.34		1.00				C
MOTA	2215	CD1					271	32.4		25.82		L.00				C
MOTA	2216	CD2					701	31.0		27.86		L.00				C
ATOM	2217		ASN A				909	26.8		26.12		1.00				N
MOTA	2218		ASN A				890	25.9		25.70		1.00				C
MOTA	2219		ASN A				373	24.9		24.66		1.00				C
MOTA	2220		ASN A				593	24.4		23.83		1.00				0
MOTA	2221		ASN 3				283	26.7		25.19		1.00				C C
ATOM	2222		ASN A				805	27.7		26.25		1.00				0
ATOM	2223		ASN A				266	27.3		27.31 25.97		1.00				И
MOTA	2224		ASN :				716 648	29.0		24.73		1.00				N
ATOM	2225		GLY .				220	23.5		23.80		1.00				C
ATOM	2226		GLY				556	22.2		24.42		1.00				Č
ATOM ATOM	2227 2228		GLY				071	21.3		23.76		1.00				ŏ
ATOM	2229		GLY			•	255	22.1		25.70		1.00				N
ATOM	2230	CA	GLY				521	20.8		26.37		1.00				C
MOTA	2231	C.	GLY				964	20.		26.76		1.00				C
ATOM	2232	ŏ	GLY				727	21.		26.52		1.00				0
ATOM	2233	N	ILE				.351	19.		27.3		1.00	34.5	55		N
ATOM	2234	CA	ILE				. 671	19.		27.9		1.00				С
ATOM	2235	C	ILE				.702	19.		26.83		1.00	34.8	37		С
ATOM	2236	0	ILE			7	.417	19.	196	25.6	87	1.00	35.2	21		0
ATOM	2237	CB	ILE			6	.815	18.	325	28.7	86		35.0		•	С
MOTA	2238	CG1	ILE			7	.018	17.	091	27.9	24	1.00	35.3	30	•	С
MOTA	2239	CG2	ILE	Α	289	5	.610	18.	143	29.6	94	1.00	35.2	22		С
MOTA	2240	CD1	ILE	A	289	7	.654	15.	972	28.6	98		· 35.			С
MOTA	2241	N	THR				.921	19.		27.2			34.			N
ATOM	2242	CA	THR			10	.001	19.		26.2			34.		•	С
ATOM	2243	С	THR				.103	18.		26.7			34.			C
MOTA	2244	0			290		.286	18.		27.9			34.			0
MOTA	2245	СВ			290		.522	21.		26.0			34.			C
MOTA	2246		THR				.747		863	27.3			34.			0 C
MOTA	2247		THR				.455		105	25.4			34.			
ATOM	2248	N					.832			25.8			33.			И С
MOTA	2249	CA			291		.940		576	26.1			34. 33.			·C
ATOM	2250	C			291		.091		963 203	25.3 24.1			33.			0
ATOM	2251 2252	O			291 291		.933 .590		111	26.0			34.		•	c
ATOM ATOM	2252	CB	ILE				.439		793	26.9			34.			č
ATOM	2254		ILE				.758		248	26.4			34.			Č
ATOM	2255		ILE				021		384	26.9			35.			Ċ
ATOM	2256				292		.254		062	25.9			33.			N
ATOM	2257	CA			292		5.410		418	25.1			33.			C
ATOM	2258				292		1.579		741	25.7			33.			С
ATOM	2259				292		623		472				33.			0
ATOM	2260				292		5.725		921				33.			С
ATOM	2261		THR				5.590		725				33.			0
ATOM	2262		THR				7.774		293				34.			С
ATOM	2263				293		3.565		518			1.00	34.	.13		N
MOTA	2264				293		9.821		.030		391		34.			С
ATOM	2265		VAL	A	293	20	0.935	17	. 867				0 34.			С
MOTA	2266	0			293		1.039		.017				0 34.			0
MOTA	2267	_ CB	VAI	, A	293	20	0.029	15	. 603	25.0	019	1.0	0 34	. 66		С

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MOTA	2268	CG1	VAL A	293	21.473	15.238	25.222	1.00	35.24		С
ATOM	2269	CG2	VAL A	293	19.141	14.741	25.880		35.15		C
ATOM	2270	N	ASN A		21.768	18.433	25.681		34.82		И
MOTA	2271	CA	ASN A		22.890	19.187	25.174		34.61		C
ATOM	2272	С	ASN A		24.159	18.372	25.251		34.68		C
ATOM	2273	0	ASN A		24.220	17.350	25.934		34.28		
ATOM	2274	CB	ASN A		23.036	20.571	25.829		34.77		O C
ATOM	2275	CG	ASN A		23.676	20.533	27.197		33.90		
ATOM	2276		ASN A		24.170	19.504	27.653		36.35		C
ATOM	2277		ASN A		23.658	21.670	27.868		30.46		0
MOTA	2278	N	PHE A		25.141	18.870	24.510		34.93		N
MOTA	2279	CA	PHE A		26.450	18.291	24.326		35.27		И
ATOM	2280	C	PHE A		27.467	19.411	24.552		35.69		С
ATOM	2281	Õ	PHE A		27.610	20.288	23.698		35.68		С
ATOM	2282	СВ	PHE A		26.581	17.832	22.875		35.88		0
ATOM	2283	CG	PHE A		25.858	16.554	22.545		34.85		C
ATOM	2284		PHE A		24.492	16.549	22.332		35.36		
ATOM	2285		PHE A		26.559	15.371	22.383		33.46		C .
ATOM	2286		PHE A		23.841	15.371	21.996		35.19		C.
ATOM	2287		PHE A		25.918	14.207	22.048				С
ATOM	2288		PHE A		24.566	14.202			33.20		C
ATOM	2289	N	TRP A		28.182		21.853		34.09		С
ATOM	2290	CA	TRP A		29.113	19.369 20.433	25.677		36.18		N
ATOM	2291	C	TRP A		30.534		26.073		36.34		C
ATOM	2292	Ö	TRP A		30.932	19.963	25.938		36.50		С
ATOM	2293	СВ	TRP A			18.969	26.563		36.32		0
ATOM	2294	CG	TRP A		28.913 27.934	20.830	27.541		36.57		C.
ATOM	2295	CD1				21.912	27.776		37.38		C
ATOM	2296	CD2			26.997	22.361	26.909		38.36		С
ATOM	2297	NE1			27.787	22.693	28.965		39.42		С
ATOM	2298		TRP A		26.275	23.384	27.473		38.20		N
ATOM	2299		TRP A		26.737	23.605	28.736		38.86		С
ATOM	2300		TRP A		28.450	22.730	30.204		40.74		С
ATOM	2301		TRP A		26.327	24.529	29.682		41.03		С
ATOM	2302		TRP A		28.037	23.665	31.160		40.86		С
ATOM	2302	N	TYR A		26.989	24.544	30.891		41.52		С
ATOM	2304	CA			31.303	20.719	25.162		36.60		N
ATOM	2304	CA	TYR A		32.703	20.442	24.923		36.79		С
ATOM	2306	0	TYR A		33.534	21.597	25.457		36.96		C
ATOM	2307	СВ	TYR A		33.117	22.734	25.363		36.32		0
ATOM	2308	CG	TYR A		32.923	20.291	23.423		36.93		C
MOTA	2309		TYR A		32.280	19.054	22.868		37.30		С
ATOM	2310		TYR A		30.939	19.046	22.523		37.28		С
ATOM	2311		TYR A		33.008	17.880	22.716		36.72		С
ATOM	2312				30.346	17.907	22.039		37.15		С
ATOM	2312		TYR A		32.423	16.747	22.226		35.89		С
ATOM		CZ	TYR A		31.088		21.893		36.57		С
ATOM	2314 2315	OH	TYR A		30.467	15.641	21.405		36.99		0
ATOM		N	LYS A		34.696	21.303	26.039		37.93		N
	2316	CA	LYS A		35.615	22.347	26.495		38.45		С
MOTA	2317	C	LYS A		36.090	22.994	25.236		38.43		С
ATOM	2318	0	LYS A		36.245	22.320	24.229		38.55		0
MOTA	2319	CB	LYS A		36.835	21.782	27.233		38.67		С
MOTA	2320	CG	LYS A		36.634	21.550	28.737		40.58		C
MOTA	2321	CD	LYS A		37.928	21.093	29.484		42.63		С
MOTA	2322	CE	LYS A		37.631	20.622	30.951		44.00		C
ATOM	2323	NZ	LYS A		38.841	20.251	31.812		43.61		N
MOTA	2324	N	GLY A		36.347	24.286	25.277		38.82		N
MOTA	2325	CA	GLY A		36.768	24.976	24.080		39.19		С
MOTA	2326	С	GLY A		38.174	24.582	23.719		39.60		С
ATOM	2327	0	GLY A		38.859	23.930	24.502		39.93		0
MOTA	2328	N	ALA A	300	38.594	24.963	22.520	1.00	40.20		N

ATOM	2329	CA .	ALA Z	A :	300	39.9	963	24.751	22.072	1.00	40.70	С	
MOTA			ALA Z			40.9		25.588	22.929		41.18	С	
MOTA			ALA A			40.4	183	26.417	23.722	1.00	41.25	0	
MOTA	2332	CB .	ALA	A	300	40.0	085	25.143	20.616	1.00	40.64	С	
MOTA	2333	N	PRO 2	Α	301	42.	215	25.408	22.733	3 1.00	41.91	N	
MOTA	2334	CA	PRO :	A	301	43.	213	26.102	23.542	2 1.00	42.49	С	
MOTA	2335	С	PRO .	Α	301	43.	448	27.541	23.128	3 1.00	43.14	С	
MOTA	2336	0	PRO .	A	301	43.		27.899	21.962	2 1.00	43.31	0	
MOTA	2337	CB	PRO	Α	301	44.	483	25.326	23.23		42.38	C	
MOTA	2338	CG	PRO	Α	301	44.	300	24.924	21.83		42.16	С	
MOTA	2339	CD	PRO			42.		24.571	21.70		41.99	С	
ATOM	2340	N	THR			43.		28.343	24.11		43.86	N	
MOTA	2341	CA	THR			44.		29.726	23.91		44.26	C	
MOTA	2342	С	THR			45.		29.732	23.31		44.56	C	
ATOM	2343	0	THR				524	29.337	24.01		44.82	0	
ATOM	2344	CB	THR				284	30.383	25.27		44.20	C	
MOTA	2345		THR				030	30.253	25.95	•	45.23	0	
ATOM	2346		THR				512	31.858	25.13		44.53	C	
MOTA	2347	N	PRO				770	30.229	22.09		44.72	И С	
ATOM	2348	CA	PRO				083	30.128	21.43		44.51		
ATOM	2349	C	PRO				177	30.759 31.522	22.30		44.48 44.02	0	
ATOM	2350	O	PRO				835	30.929	23.22		44.55	c	
MOTA.	2351	CB			303		897 426	30.929	20.14 19.90		44.28	C	
ATOM	2352 2353	CG CD			303 303		834	31.040	21.28		44.71	· · · · · · · · · · · · · · · · · · ·	
MOTA MOTA	2354	И			307		829	36.983	18.73		42.48	И	
ATOM	2355	CA			307		845	37.952	17.64		42.70	c	
ATOM	2356	C			307		812	39.039	17.80		42.57	Ċ	
ATOM	2357	o			307		654	38.807	18.13		42.62	Ö	
ATOM	2358	СВ			307		624	37.296	16.28		43.00	Ċ	
ATOM	2359	CG			307		980	38.235	15.12		43.85	C	
MOTA	2360	CD			307		.091	37.541	13.77		44.71	C	2
ATOM	2361				307		618	36.385			45.10	C	
ATOM	2362	OE2			307		. 649	38.170			45.60	C)
ATOM	2363	N			308		.249	40.243			42.66	N	Į
ATOM .	2364	CA			308		.384	41.379		77 1.00	42.64	C	
MOTA	2365	С			308	. 44	.814	41.530	16.18	39 1.00	42.85	C	
ATOM	2366	0	TYR	. A	308		.413	41.066	15.20	3 1.00	43.43		2
MOTA	2367	CB	TYR	. A	308	. 46	.184	42.565	18.03	34 1.00	42.47	C	3
MOTA	2368	CG	TYR	A	308	46	.744	42.281	19.39	99 1.00	43.35	(C
MOTA	2369	CD1	TYR	A	308	45	.996	42.552			44.58		C
MOTA	2370	CD2	TYR	A	308		.986				43.97		С
MOTA	2371				308		.482	42.284			45.23		C
MOTA	2372				308		.483	41.401			44.79		С
MOTA	2373	CZ			308		.726	41.708			45.46		С
MOTA	2374	OH			308		.200	41.453			45.86		0
MOTA	2375	N			A 309		. 631	42.119			42.47		N
MOTA	2376	CA			309		.930	42.648			42.08		C
MOTA	2377	С			309		.209	41.528			11.24		C
MOTA	2378	0			309		.774	40.578			0 40.92		0
ATOM	2379	СВ			A 309		.910	43.583			0 42.39		C
MOTA	2380	CG			A 309		.574	42.895			0 42.16		C
ATOM	2381				A 309		.843	42.260			0 42.28		C
ATOM	2382				A 310		.059	41.654			0 40.25		N
ATOM	2383				A 310		.436				0 39.46		C C
ATOM	2384				A 310		971				0 38.93 0 39.65		o
ATOM	2385				A 310 A 310		.288 .526				0 39.63		c
ATOM	2386 2387				A 310		486				0 39.21		c
ATOM ATOM	2388				A 310		3.727				0 38.58		c
ATOM	2389				A 310		2.817				0 30.30		c
ATON	2303	- UD	الالبات	- 1		7.4			. 23.1	1.0			_

ATOM	2390	N	LYS. A	311	39.462	39.217	19.957	1.00 37.90	N
MOTA	2391	CA	LYS A	311	38.036	39.029	19.731	1.00 37.53	С
MOTA	2392		LYS A		37.217	39.359	20.978	1.00 36.85	С
MOTA	2393		LYS A		37.705	39.272	22.092	1.00 36.85	0
ATOM	2394		LYS A		37.746	37.609	19.274	1.00 37.54	С
ATOM	2395		ALA A		35.965	39.736	20.793	1.00 36.18	N
MOTA	2396	CA	ALA A		35.112	40.015	21.937	1.00 35.92	C
ATOM	2397	С	ALA A		35.232	38.994	23.058	1.00 35.88	C
ATOM ATOM	2398 2399	O CB	ALA A		35.347 33.665	39.384 40.115	24.213	1.00 35.99 1.00 35.50	0 C
ATOM	2400	N	HIS A		35.221	37.700	21.526 22.739	1.00 35.30	N
ATOM	2400	CA	HIS A		35.136	36.709	23.797	1.00 35.71	C
ATOM	2402	C	HIS A		36.429	36.694	24.517	1.00 35.32	Ċ
ATOM	2403	Ö	HIS A		36.489	36.278	25.667	1.00 35.53	Ö
ATOM	2404	СВ	HIS A		34.768	35.291	23.313	1.00 35.89	Č
ATOM	2405	CG	HIS A		35.844	34.613	22.535	1.00 36.41	С
ATOM	2406	ND1	HIS A	313	36.097	34.905	21.214	1.00 38.71	N
MOTA	2407		HIS A		36.741	33.665	22.889	1.00 37.90	С
MOTA	2408		HIS A		37.111	34.175	20.789	1.00 38.65	C
MOTA	2409		HIS A		37.524	33.416	21.788	1.00 38.60	. N
MOTA	2410	N	GLN A		37.478	37.162	23.861	1.00 35.08	
ATOM	2411	CA	GLN A		38.760	37.203	24.535	1.00 35.00	C
ATOM	2412	C	GLN A		38.706	38.301	25.576	1.00 34.62	C
ATOM ATOM	2413 · 2414	O	GLN A		39.145	38.109	26.703	1.00 34.28	0
ATOM	2414	CB CG	GLN A		39.924 40.091	37.399 36.229	23.558 22.597	1.00 35.10 1.00 35.42	C C
ATOM	2415	CD	GLN A		41.107	36.478	21.500	1.00 35.42	C
ATOM	2417		GLN A		40.938	37.377	20.671	1.00 35.10	Ö
ATOM	2418		GLN A		42.150	35.666	21.476	1.00 34.32	N
ATOM	2419	N	LYS A		38.173	39.454	25.197	1.00 34.70	N
MOTA	2420	CA	LYS A		38.009	40.539	26.152	1.00 35.01	С
MOTA	2421	C	LYS A	315	37.164	40.063	27.320	1.00 34.67	С
MOTA	2422	0	LYS F	315	37.485	40.325	28.467	1.00 34.81	0
MOTA	2423	CB	LYS A		37.395	41.766	25.501	1.00 35.19	С
ATOM	2424	CG	LYS F		38.344	42.447	24.563	1.00 35.85	С
ATOM	2425	CD	LYS A		37.703	43.636	23.931	1.00 37.25	C
ATOM	2426	CE	LYS A		38.657	44.348	23.001	1.00 39.28	C
ATOM ATOM	2427 2428	NZ	LYS A		37.969	45.430	22,222	1.00 40.34	N
ATOM	2429	N CA	VAL A		36.117 35.321	39.314 38.787	27.040 28.118	1.00 34.30 1.00 34.31	N C
ATOM	2430	C	VAL A		36.175	37.925	29.047	1.00 34.37	C
ATOM	2431	Ö	VAL A		36.071	38.023	30.273	1.00 34.57	. 0
ATOM	2432	СВ		A 316	34.138	37.992	27.606	1.00 34.39	C
MOTA	2433		VAL A		33.334	37.434	28.794	1.00 34.91	C
ATOM	2434		VAL A		33.258	38.873	26.719	1.00 33.60	С
MOTA	2435	N	ALA A	A 317	37.011	37.072	28.475	1.00 34.24	N
MOTA	2436	CA		A 317	37.907	36.267	29.288	1.00 34.17	C
MOTA	2437	С		A 317 _.	. 38.744	37.160	30.166	1.00 34.10	С
MOTA	2438	0		A 317	38.919	36.906	31.352	1.00 33.87	0
ATOM	2439	CB		A 317	38.813	35.459	28.431	1.00 34.02	C
ATOM	2440	N		A 318	39.274	38.216	29.574	1.00 34.29	N
ATOM ATOM	2441	CA		A 318	40.178	39.062	30.322	1.00 34.26	C
ATOM	2442 2443	C O		A 318 A 318	39.467 39.993	39.611 39.556	31.546 32.661	1.00 33.99 1.00 33.96	C 0
ATOM	2443	СВ		A 318	40.755	40.171	29.447	1.00 33.98	c
ATOM	2445		ILE A		41.775	39.558	28.489		C
ATOM	2446		ILE :		41.429	41.188	30.323	1.00 34.02	, c
ATOM	2447		ILE		42.356	40.498	27.428	1.00 33.97	Ċ
MOTA	2448	N		A 319	38.241	40.068	31.337	1.00 33.55	N
MOTA	2449		MET .	A 319	37.499	40.741	32.383	1.00 33.41	С
MOTA	2450	C	MET .	A 319	37.196	39.772	33.496	1.00 33.38	C

B.MON	0453	^	METER A	210	37.238	40.101	34.669	1.00 33.32	0
ATOM	2451		MET A						c
ATOM	2452		MET A		36.193	41.308	31.827	1.00 33.31	c
MOTA	2453		MET A		36.361	42.521	30.951	1.00 32.96	
ATOM	2454		MET A		34.812	43.355	30.617	1.00 33.05	S ·
MOTA	2455	CE	MET A		34.119	42.299	29.410	1.00 33.43	C
MOTA	2456	N	ARG A		36.873	38.558	33.121	1.00 33.68	N
ATOM	2457	CA	ARG A	320	36.575	37.568	34.112	1.00 33.61	С
ATOM	2458	С	ARG A	320	37.796	37.392	34.996	1.00 33.82	С
ATOM	2459	0	ARG A	320	37.719	37.448	36.225	1.00 33.48	0
MOTA	2460	CB	ARG A		36.211	36.292	33.402	1.00 33.39	С
MOTA	2461	CG	ARG A		34.875	36.406	32.725	1.00 33.88	С
ATOM	2462	CD	ARG A		34.268	35.080	32.340	1.00 34.20	С
ATOM	2463	NE	ARG A		34.217	34.215	33.507	1.00 33.14	N
ATOM	2464	CZ	ARG A		33.159	34.103	34.260	1.00 33.15	С
ATOM	2465		ARG A		32.077	34.762	33.933	1.00 33.83	N
					33.170	33.338	35.331	1.00 33.03	N
ATOM	2466		ARG A					1.00 33.92	N
ATOM	2467	N	ASN A		38.941	37.232	34.355		C
ATOM	2468	CA	ASN A		40.143	36.978	35.085	1.00 34.08	
MOTA	2469	С	ASN A		40.486	38.141	36.018	1.00 34.26	C
MOTA	2470	0	ASN A		40.874		37.164	1.00 34.14	. 0
MOTA	2471	CB	ASN A		41.271	36.616	34.119		C
MOTA	2472	CG	ASN F		41.195	35.161	33.663	1.00 34.44	С
MOTA	2473	OD1	ASN A	321	40.829	34.273	34.434	1.00 34.16	0
MOTA	2474	ND2	ASN A	321	41.522	34.918	32.402	1.00 35.05	N
ATOM	2475	N	ILE A	A 322	40.318	39.379	35.569	1.00 34.24	N
ATOM	2476	CA	ILE A	A 322	40.634	40.488	36.448	1.00 34.25	C
ATOM	2477	С		A 322	39.781	40.408	37.701	1.00 33.85	С
ATOM	2478	Ō		A 322	40.250	40.711	38.789	1.00 34.16	0
ATOM	2479	СВ		A 322	40.412	41.837	35.760	1.00 34.70	С
ATOM	2480	CG1		A 322	41.338	41.993	34.558	1.00 35.34	C
ATOM	2481		ILE A		40.651	43.007	36.748	1.00 35.37	Ċ
ATOM	2482		ILE A		42.778	41.928	34.895	1.00 36.17	Č
									N
ATOM	2483	N		A 323	38.525	40.013	37.558	1.00 33.42	C
ATOM	2484	CA		A 323	37.636	39.935	38.704	1.00 32.97	C
ATOM	2485	C		A 323	38.085	38.842	39.652	1.00 33.11	
ATOM	2486	0		A 323	38.067	39.001	40.864	1.00 32.66	0
ATOM	2487	CB		A 323	36.199	39.673	38,256	1.00 32.73	C
MOTA	2488	CG		A 323	35.543	40.907	37.672	1.00 33.02	C
ATOM	2489	CD		A 323	34.166	40.693	37.057	1.00 32.91	C
ATOM	2490		GLU .		33.193	40.309	37.740	1.00 31.94	0
MOTA	2491				34.048	40.961	35.856	1.00 33.81	0
MOTA,	2492	N	LYS	A 324	38.497	37.720	39.088		N
ATOM	2493	CA	LYS	A 324	38.882	36.588	39.895	1.00 33.72	С
MOTA	2494	C	LYS	A 324	40.138	36.937	40.670	1.00 34.09	С
MOTA	2495	0	LYS	A 324	40.228	36.664	41.859	1.00 34.15	0
MOTA	2496	CB	LYS	A 324	39.119	35.368	39.012	1.00 33.73	С
ATOM	2497	CG		A 324	37.877	34.766	38.353	1.00 33.83	C
MOTA	2498	CD		A 324		33.673	37.440		С
MOTA	2499			A 324	37.294		36.723		С
MOTA	2500			A 324	37.993	31.761			N
ATOM	2501			A 325	41.098		39.995		N
MOTA	2502			A 325	42.380		40.609		C
					42.248				Č
MOTA	2503			A 325		38.883	41.766		0
ATOM	2504			A 325	42.888	38.729			
MOTA	2505			A 325	43.328	38.501	39.563		C
MOTA	2506			A 325	43.962				C
ATOM	2507			A 325	44.984				S
ATOM	2508			A 325	45.710				С
ATOM	2509			A 326	41.427				N
MOTA	2510			A 326	41.178				C
MOTA	2511	. С	LEU	A 326	40.556	40.230	43.770	1.00 35.60	С

ATOM 2512 O LBU A 326											• • • • •	
ATOM 2513 CB LEU A 326 40.216 41.929 42.026 1.00 36.07 ATOM 2515 CG LEU A 326 40.721 43.321 41.699 1.00 37.48 ATOM 2515 CD LEU A 326 42.221 43.442 41.537 1.00 38.65 ATOM 2516 CD2 LEU A 326 42.221 43.442 41.537 1.00 38.65 ATOM 2516 CD2 LEU A 326 40.049 43.692 40.413 1.00 38.65 ATOM 2510 CA GLY A 327 39.613 39.341 43.493 1.00 38.55 ATOM 2510 CA GLY A 327 39.963 37.998 45.443 1.00 38.55 ATOM 2510 CA GLY A 327 39.963 37.998 45.443 1.00 38.55 ATOM 2520 O GLY A 327 40.023 38.258 46.641 1.00 38.55 ATOM 2522 CA GLU A 328 40.863 37.209 44.851 1.00 38.55 ATOM 2522 CA GLU A 328 40.863 37.209 44.851 1.00 38.57 ATOM 2522 CA GLU A 328 41.831 36.486 45.632 1.00 38.51 ATOM 2523 C GG LU A 328 42.783 37.424 46.298 1.00 38.54 ATOM 2525 CB GLU A 328 42.584 35.513 44.750 1.00 38.62 ATOM 2525 CB GLU A 328 42.584 35.513 44.750 1.00 38.62 ATOM 2525 CB GLU A 328 41.675 34.419 44.226 1.00 38.62 ATOM 2527 CD GLU A 328 41.675 34.419 44.226 1.00 38.62 ATOM 2527 CD GLU A 328 41.675 34.419 44.226 1.00 38.20 ATOM 2527 CD GLU A 328 41.675 34.419 44.226 1.00 38.20 ATOM 2527 CD GLU A 328 41.675 34.419 44.226 1.00 38.20 ATOM 2527 CD GLU A 328 41.675 34.419 44.226 1.00 38.20 ATOM 2527 CD GLU A 328 41.675 34.419 44.226 1.00 38.20 ATOM 2529 CEZ GLU A 328 41.675 34.419 44.226 1.00 38.21 ATOM 2520 CD GLU A 328 41.675 34.419 44.226 1.00 38.23 ATOM 2520 CD GLU A 328 41.675 34.419 44.226 1.00 38.23 ATOM 2530 N ALA 329 44.259 39.282 46.110 1.00 34.65 ATOM 2531 CA ALA A 329 44.259 39.282 46.110 1.00 34.65 ATOM 2531 CA ALA A 329 44.579 41.204 41.205 1.00 34.55 ATOM 2531 CA ALA A 329 44.579 41.204 41.205 1.00 34.55 ATOM 2531 CA ALA A 329 44.579 41.204 41.205 1.00 34.55 ATOM 2531 CA ALA A 329 44.579 39.282 46.110 1.00 34.65 ATOM 2531 CA ALA A 329 44.579 39.282 46.110 1.00 34.65 ATOM 2531 CA ALA A 329 44.579 39.282 46.110 1.00 34.65 ATOM 2531 CA ALA A 329 44.778 40.153 40.282 40.743 41.00 34.65 ATOM 2531 CA ALA A 329 44.778 40.153 40.282 40.743 41.00 34.65 ATOM 2540 CB LEU A 330 41.244 41.00 34.62 ATOM 2551 CB ALA A 329 44.778 41.00 41.00 34.62 ATOM 2551 CB AL							40.914	40.507	44.910	1.00 35.34		0
ATCOM 2515 CD1 LEU A 326							40.216	41.929				C
ATOM 2515 CD LEU A 326							40.721	43.321				č
ATOM 2517 N G LY A 327 39,613 39,341 43,493 1.00 38,65 ATOM 2518 CA GLY A 327 38,613 43,692 40,413 1.00 35,59 ATOM 2518 CA GLY A 327 38,6947 38,604 44,538 1.00 35,54 ATOM 2520 O GLY A 327 40,023 38,258 46,641 1.00 35,52 ATOM 2521 N GLU A 328 40,863 37,209 44,851 1.00 35,52 ATOM 2522 CA GLU A 328 40,863 37,209 44,851 1.00 35,59 ATOM 2523 C GLU A 328 42,783 37,984 46,298 1.00 35,91 ATOM 2524 O GLU A 328 42,783 37,424 46,298 1.00 35,91 ATOM 2525 CG GLU A 328 42,544 35,513 44,750 1.00 36,60 ATOM 2525 CG GLU A 328 41,675 34,419 44,226 1.00 36,60 ATOM 2526 CG GLU A 328 41,675 34,419 44,226 1.00 38,20 ATOM 2528 OEI GLU A 328 41,675 34,419 44,226 1.00 34,43 ATOM 2528 OEI GLU A 328 41,675 34,419 44,226 1.00 34,40 ATOM 2528 OEI GLU A 328 42,544 33,084 46,138 1.00 42,40 ATOM 2530 N ALA A 329 43,220 38,435 45,577 1.00 34,50 ATOM 2530 N ALA A 329 44,259 39,282 46,110 1.00 34,85 ATOM 2532 C ALA A 329 44,259 39,282 46,110 1.00 34,85 ATOM 2532 C ALA A 329 44,259 39,282 46,110 1.00 34,85 ATOM 2533 O ALA A 329 44,259 39,282 46,110 1.00 34,85 ATOM 2533 O ALA A 329 44,259 39,282 46,110 1.00 34,85 ATOM 2535 N BLU A 330 42,567 A 0,163 47,296 1.00 34,53 ATOM 2535 N BLU A 330 42,567 A 0,163 47,296 1.00 34,53 ATOM 2535 N BLU A 330 41,478 40,163 47,296 1.00 34,53 ATOM 2538 O LEU A 330 41,478 40,163 47,296 1.00 34,53 ATOM 2538 O LEU A 330 41,478 40,163 47,296 1.00 34,53 ATOM 2539 C BLU A 330 41,478 40,155 49,448 1.00 34,62 ATOM 2539 C BLU A 330 41,478 40,155 49,448 1.00 34,62 ATOM 2534 CB LEU A 330 41,296 41,399 39,262 49,232 1.00 35,23 ATOM 2540 CG LEU A 330 41,294 41,295 39,262 49,232 1.00 35,66 ATOM 2540 CG LEU A 330 41,294 41,072 50,592 1.00 36,56 ATOM 2540 CG LEU A 330 41,294 41,295 39,262 49,232 1.00 36,56 ATOM 2540 CG LEU A 330 41,294 41,295 39,262 49,232 1.00 36,64 ATOM 2540 CG LEU A 330 39,942 43,955 46,258 1.00 34,23 ATOM 2540 CG LEU A 330 41,294 41,295 39,262 49,232 1.00 36,64 ATOM 2550 CG RN A 333 34,148 41,097 50,194 1.00 36,56 ATOM 2551 CR ASN A 332 36,647 39,947 41,949 41,092 61,00 36,56 ATOM 2555 CG RN A 333 34,148 41,094							42.221	43.442	41.537			Č
ATOM 2518 CA GLY A 327 38, 943 39, 341 43, 493 1.00 35, 59 ATOM 2519 C GLY A 327 38, 983 37, 998 45, 443 1.00 35, 62 ATOM 2520 O GLY A 327 40, 023 38, 258 46, 641 1.00 35, 62 ATOM 2521 N GLU A 328 40, 863 37, 209 44, 851 1.00 35, 84 ATOM 2522 CA GLU A 328 41, 831 36, 486 45, 632 1.00 35, 84 ATOM 2523 C GLU A 328 42, 783 37, 424 46, 298 1.00 35, 44 ATOM 2524 O GLU A 328 42, 783 37, 424 46, 298 1.00 35, 44 ATOM 2525 CB GLU A 328 42, 584 35, 513 44, 750 1.00 36, 21 ATOM 2525 CB GLU A 328 42, 584 35, 513 44, 750 1.00 36, 21 ATOM 2526 CG GLU A 328 41, 854 33, 088 44, 941 1.00 41, 33 ATOM 2527 CD GLU A 328 41, 854 33, 088 44, 941 1.00 41, 33 ATOM 2529 OE2 GLU A 328 41, 854 33, 084 46, 138 1.00 42, 40 ATOM 2530 N ALA A 329 41, 200 38, 435 45, 577 1.00 35, 11 ATOM 2531 CA ALA A 329 44, 259 39, 282 46, 110 1.00 34, 59 ATOM 2531 CA ALA A 329 44, 259 39, 282 46, 110 1.00 34, 75 ATOM 2533 N ALA A 329 44, 259 39, 282 48, 258 1.00 34, 75 ATOM 2533 O ALA A 329 44, 778 40, 163 45, 046 1.00 34, 85 ATOM 2533 N ALB A 329 44, 778 40, 163 45, 046 1.00 34, 85 ATOM 2535 N EU A 330 41, 996 41, 399 48, 291 1.00 34, 53 ATOM 2536 C B GLU A 330 41, 296 40, 139 48, 291 1.00 34, 55 ATOM 2537 C EU A 330 41, 296 41, 399 48, 291 1.00 34, 62 ATOM 2538 O LEU A 330 41, 296 41, 399 48, 291 1.00 34, 62 ATOM 2537 C LEU A 330 41, 296 41, 399 48, 291 1.00 34, 62 ATOM 2537 C LEU A 330 41, 296 41, 399 48, 291 1.00 34, 62 ATOM 2540 CG LEU A 330 41, 478 40, 156 46, 296 1.00 34, 62 ATOM 2540 CG LEU A 330 41, 478 40, 157 50, 532 1.00 35, 33 ATOM 2540 CG LEU A 330 41, 296 41, 399 48, 291 1.00 34, 62 ATOM 2540 CG LEU A 330 41, 478 40, 157 50, 532 1.00 35, 33 ATOM 2540 CG LEU A 330 41, 294 41, 292 43, 955 51, 544 41, 00 34, 62 ATOM 2540 CG LEU A 330 41, 478 40, 157 50, 532 1.00 35, 23 ATOM 2540 CG LEU A 330 41, 294 41, 292 41, 292 1.00 36, 64 ATOM 2540 CG LEU A 330 41, 478 40, 555 50, 504 40, 600 35, 600 36, 60							40.049	43.692	40.413			Č
ATOM 2518 C A GLY A 327 38, 947 38, 604 44,538 1.00 35,54 ATOM 2520 O GLY A 327 40,023 38,258 46,641 1.00 35,52 ATOM 2521 N GLU A 328 40,863 37,209 44,851 1.00 35,52 ATOM 2522 CA GLU A 328 41,831 36,486 45,632 1.00 35,91 ATOM 2523 C GLU A 328 42,783 37,424 46,229 1.00 35,44 ATOM 2524 O GLU A 328 42,783 37,424 46,298 1.00 35,44 ATOM 2525 CB GLU A 328 42,783 37,424 46,298 1.00 35,44 ATOM 2525 CB GLU A 328 41,675 34,419 44,750 1.00 36,21 ATOM 2526 CG GLU A 328 41,675 34,419 44,256 1.00 38,20 ATOM 2527 CD GLU A 328 41,675 34,419 44,256 1.00 38,20 ATOM 2528 OEI GLU A 328 41,675 34,419 44,256 1.00 38,20 ATOM 2529 OE2 GLU A 328 41,675 34,419 44,226 1.00 38,20 ATOM 2529 OE2 GLU A 328 41,608 32,034 44,292 1.00 43,59 ATOM 2530 N ALA A 329 43,220 38,435 45,577 1.00 35,11 ATOM 2531 CA ALA A 329 43,220 38,435 45,577 1.00 35,11 ATOM 2531 CA ALA A 329 44,259 39,282 46,110 1.00 34,85 ATOM 2533 O ALA A 329 44,533 40,282 48,258 1.00 34,55 ATOM 2533 C ALA A 329 44,533 40,282 48,258 1.00 34,55 ATOM 2535 N LEU A 330 42,567 40,613 47,296 1.00 34,55 ATOM 2535 N LEU A 330 42,567 40,613 47,296 1.00 34,55 ATOM 2535 C ALE A 329 44,533 40,282 48,258 1.00 34,55 ATOM 2535 C ALE A 339 44,533 41,998 41,918 40,163 47,214 1.00 34,62 ATOM 2535 N LEU A 330 41,996 41,399 48,291 1.00 34,55 ATOM 2535 N LEU A 330 41,996 41,399 48,291 1.00 34,55 ATOM 2536 CA LEU A 330 41,478 40,555 49,448 1.00 34,62 ATOM 2537 C LEU A 330 41,478 40,555 49,448 1.00 34,62 ATOM 2539 CB LEU A 330 41,294 41,778 40,163 47,214 1.00 34,62 ATOM 2539 CB LEU A 330 41,294 41,798 40,555 49,448 1.00 34,06 ATOM 2541 CDI LEU A 330 41,294 41,798 40,555 49,448 1.00 34,06 ATOM 2541 CDI LEU A 330 41,294 41,798 40,163 47,244 1.00 34,06 ATOM 2541 CDI LEU A 330 41,294 41,798 40,155 40,494 41,494								39.341	43.493			N
ATOM 2519 C GLY A 327							38.947	38.604	44.538			C
ATOM 2521 N GLY A 327 40,023 38,258 46,641 1.00 35,52 ATOM 2522 CA GLU A 328 41,831 37,029 44,851 1.00 35,91 ATOM 2523 C GLU A 328 41,831 37,424 46,298 1.00 35,91 ATOM 2524 O GLU A 328 42,783 37,424 46,298 1.00 35,60 ATOM 2525 CB GLU A 328 42,784 35,513 44,750 1.00 36,21 ATOM 2526 CG GLU A 328 42,584 35,513 44,750 1.00 36,21 ATOM 2526 CG GLU A 328 41,854 35,088 44,941 1.00 41,33 ATOM 2527 CD GLU A 328 41,854 33,088 44,941 1.00 41,33 ATOM 2528 OEI GLU A 328 41,854 33,088 44,941 1.00 41,33 ATOM 2529 OE2 GLU A 328 41,854 33,088 44,941 1.00 41,33 ATOM 2520 OE2 GLU A 328 41,854 33,088 44,941 1.00 41,33 ATOM 2520 OE2 GLU A 328 41,854 33,088 44,941 1.00 41,33 ATOM 2530 OR ALA A 329 44,259 39,282 46,110 1.00 34,85 ATOM 2531 CA ALA A 329 44,259 39,282 46,110 1.00 34,85 ATOM 2532 C ALA A 329 44,753 40,282 48,258 1.00 34,53 ATOM 2531 CB ALA A 329 44,753 40,282 48,258 1.00 34,53 ATOM 2535 N LEU A 330 42,567 40,613 47,296 1.00 34,55 ATOM 2535 N LEU A 330 42,567 40,613 47,244 1.00 34,62 ATOM 2535 N LEU A 330 42,567 40,613 47,244 1.00 34,62 ATOM 2536 CA LEU A 330 41,478 40,163 47,244 1.00 34,62 ATOM 2537 C LEU A 330 41,478 40,163 47,244 1.00 34,62 ATOM 2538 C LEU A 330 41,478 40,555 49,448 1.00 34,90 ATOM 2539 CB LEU A 330 41,296 41,399 48,291 1.00 34,55 ATOM 2539 CB LEU A 330 41,296 41,399 48,291 1.00 34,55 ATOM 2540 CG LEU A 330 41,292 43,352 47,766 1.00 34,05 ATOM 2541 CDI LEU A 330 41,292 43,955 46,258 1.00 34,05 ATOM 2541 CDI LEU A 330 41,292 43,955 46,258 1.00 34,05 ATOM 2541 CDI LEU A 330 41,292 43,955 46,258 1.00 34,05 ATOM 2541 CDI LEU A 330 41,292 43,955 46,258 1.00 34,05 ATOM 2541 CDI LEU A 330 41,292 43,955 46,258 1.00 34,05 ATOM 2541 CDI LEU A 330 41,292 43,955 46,258 1.00 34,05 ATOM 2540 CG LEU A 330 41,292 43,955 46,258 1.00 34,05 ATOM 2540 CG LEU A 330 41,292 43,955 46,258 1.00 34,05 ATOM 2540 CG LEU A 330 41,292 43,959 41,959 41,999 41,9							39.983	37.998	45.443			č
ATOM 2522 CA GLU A 328 40.863 37.209 44.851 1.00 35.84 ATOM 2523 C GLU A 328 41.831 36.466 45.632 1.00 35.91 ATOM 2525 CB GLU A 328 43.086 37.272 47.465 1.00 35.54 ATOM 2525 CB GLU A 328 43.086 37.272 47.465 1.00 35.60 ATOM 2526 CG GLU A 328 41.854 35.513 44.750 1.00 36.21 ATOM 2526 CG GLU A 328 41.854 33.088 44.941 1.00 41.33 ATOM 2527 CD GLU A 328 41.854 33.088 44.941 1.00 41.33 ATOM 2529 OEI GLU A 328 41.854 33.088 44.941 1.00 41.33 ATOM 2529 OEI GLU A 328 41.854 33.088 44.941 1.00 43.59 ATOM 2531 CA ALA A 329 44.259 39.282 46.110 1.00 36.11 ATOM 2531 CA ALA A 329 44.559 39.282 46.110 1.00 34.85 ATOM 2532 C ALA A 329 44.559 39.282 46.110 1.00 34.85 ATOM 2533 O ALA A 329 44.778 40.163 47.296 1.00 34.53 ATOM 2536 CA LEU A 330 41.996 41.399 48.291 1.00 34.53 ATOM 2537 C LEU A 330 41.996 41.399 48.291 1.00 34.55 ATOM 2537 C LEU A 330 41.996 41.399 48.291 1.00 34.55 ATOM 2539 CB LEU A 330 41.996 41.399 48.291 1.00 34.55 ATOM 2539 CB LEU A 330 41.996 41.399 48.291 1.00 34.55 ATOM 2536 CA LEU A 330 41.996 41.399 48.291 1.00 34.55 ATOM 2538 O LEU A 330 41.996 41.399 48.291 1.00 34.55 ATOM 2538 O LEU A 330 41.996 41.399 48.291 1.00 34.55 ATOM 2538 O LEU A 330 41.996 41.399 48.291 1.00 34.55 ATOM 2536 CA LEU A 330 41.996 41.399 48.291 1.00 34.55 ATOM 2537 C LEU A 330 41.996 41.399 48.291 1.00 34.55 ATOM 2540 CG LEU A 330 41.996 41.399 48.291 1.00 34.55 ATOM 2541 CD1 LEU A 330 41.996 41.399 48.291 1.00 34.55 ATOM 2540 CG LEU A 330 41.996 41.399 48.291 1.00 34.06 ATOM 2541 CD1 LEU A 330 41.996 41.399 48.291 1.00 34.06 ATOM 2541 CD1 LEU A 330 41.996 41.399 48.291 1.00 34.06 ATOM 2540 CG LEU A 330 41.996 41.399 48.291 1.00 36.61 ATOM 2551 CB LA 330 41.996 41.399 48.291 1.00 36.61 ATOM 2554 CD CLEU A 330 41.996 41.497 50.555 49.488 1.00 34.06 ATOM 2555 C C GLY A 331 38.849 37.859 51.544 1.00 34.06 ATOM 2556 C C GLY A 331 38.849 37.859 51.544 1.00 34.06 ATOM 2557 C C GLO A 333 31.40.794 38.401 50.00 36.55 ATOM 2558 C C GLY A 331 38.849 37.859 51.544 1.00 35.61 ATOM 2550 C C G RN A 333 33.41.99 39.398 46.00 37.31 ATOM 2550 C							40.023	38.258	46.641			ō
ATOM 2523 C GLU A 328 42.783 37.424 46.298 1.00 35.44 ATOM 2524 O GLU A 328 42.584 37.272 47.465 1.00 35.60 ATOM 2525 CB GLO A 328 42.584 35.513 44.750 1.00 36.21 ATOM 2526 CG GLU A 328 41.675 34.419 4.226 1.00 38.20 ATOM 2527 CD GLU A 328 41.675 34.419 4.226 1.00 38.20 ATOM 2528 OEI GLU A 328 41.675 34.419 4.226 1.00 38.20 ATOM 2528 OEI GLU A 328 41.668 32.034 44.292 1.00 42.40 ATOM 2529 OE2 GLU A 328 41.668 32.034 44.292 1.00 43.59 ATOM 2530 N ALA A 329 44.259 39.282 46.110 1.00 34.85 ATOM 2531 CA ALA A 329 44.259 39.282 46.110 1.00 34.85 ATOM 2531 CA ALA A 329 44.533 40.262 48.258 1.00 34.75 ATOM 2535 N LEU A 330 44.533 40.262 48.258 1.00 34.53 ATOM 2535 N LEU A 330 41.934 40.555 49.448 1.00 34.85 ATOM 2535 C LEU A 330 41.204 41.072 50.532 1.00 34.85 ATOM 2537 C LEU A 330 41.234 41.072 50.532 1.00 34.53 ATOM 2538 O LEU A 330 41.234 41.072 50.532 1.00 34.53 ATOM 2539 CB LEU A 330 41.234 41.072 50.532 1.00 34.55 ATOM 2538 O LEU A 330 41.234 41.072 50.532 1.00 34.55 ATOM 2538 O LEU A 330 41.234 41.072 50.532 1.00 34.55 ATOM 2538 O LEU A 330 41.234 41.072 50.532 1.00 34.55 ATOM 2538 O LEU A 330 41.202 43.322 46.743 1.00 34.62 ATOM 2541 CD1 LEU A 330 39.942 43.965 46.258 1.00 34.31 ATOM 2540 CG LEU A 330 40.851 42.245 47.766 1.00 34.05 ATOM 2541 CD1 LEU A 330 39.942 43.965 46.258 1.00 34.23 ATOM 2542 CD2 LEU A 330 39.942 43.965 46.258 1.00 34.23 ATOM 2546 C A GLY A 331 39.965 38.491 50.285 1.00 35.66 ATOM 2546 C A GLY A 331 39.965 38.491 50.285 1.00 35.61 ATOM 2546 C A GLY A 331 39.965 38.491 50.285 1.00 35.61 ATOM 2546 C A GLY A 331 39.966 38.491 50.285 1.00 35.61 ATOM 2546 C A GLY A 331 39.966 38.491 50.285 1.00 36.55 ATOM 2557 C PRO A 333 36.649 39.791 48.732 1.00 35.66 ATOM 2556 C A RO A 333 33.6649 40.959 48.991 1.00 36.64 ATOM 2557 C PRO A 333 33.36.649 39.9791 48.732 1.00 35.65 ATOM 2556 C A RO A 333 33.438 41.384 41.384 45.988 1.00 37.01 ATOM 2556 C B N A 334 33.4938 41.384 41.384 41.384 41.00 35.66 ATOM 2556 C B N A 333 33.438 34.247 77.229 47.489 1.00 36.55 ATOM 2556 C B N A 333 33.34.247 77.229 47.489									44.851	1.00 35.84		N
ATOM 2525 OB GLU A 328 42.584 37.272 47.465 1.00 33.60 ATOM 2525 CB GLU A 328 42.584 35.513 44.750 1.00 36.21 ATOM 2526 CG GLU A 328 41.675 34.419 44.226 1.00 38.20 ATOM 2527 CD GLU A 328 41.854 33.088 44.941 1.00 41.33 ATOM 2528 OEI GLU A 328 42.244 33.084 46.138 1.00 42.40 ATOM 2529 OE2 GLU A 328 41.608 32.034 44.292 1.00 43.59 ATOM 2530 N ALA A 329 43.220 38.435 45.577 1.00 35.11 ATOM 2531 CA ALA A 329 44.259 39.282 46.110 1.00 34.85 ATOM 2532 CA ALA A 329 44.259 39.282 46.110 1.00 34.85 ATOM 2533 O ALA A 329 44.533 40.282 48.258 1.00 34.75 ATOM 2534 CB ALA A 329 44.778 40.163 47.296 1.00 34.53 ATOM 2535 CA LEU A 330 42.567 40.613 47.214 1.00 34.62 ATOM 2537 C LEU A 330 41.996 41.399 48.291 1.00 34.55 ATOM 2538 O LEU A 330 41.996 41.399 48.291 1.00 34.55 ATOM 2539 CB LEU A 330 41.234 41.072 50.532 1.00 35.33 ATOM 2539 CB LEU A 330 40.851 42.245 47.766 1.00 34.90 ATOM 2539 CB LEU A 330 40.851 42.245 47.766 1.00 34.90 ATOM 2539 CB LEU A 330 41.234 41.072 50.532 1.00 35.33 ATOM 2530 CB LEU A 330 40.851 42.245 47.766 1.00 34.31 ATOM 2540 CG LEU A 330 41.204 41.072 50.532 1.00 35.33 ATOM 2540 CG LEU A 330 41.204 41.072 50.532 1.00 34.31 ATOM 2541 CDI LEU A 330 39.942 43.965 46.258 1.00 34.05 ATOM 2541 CDI LEU A 330 39.942 43.965 46.258 1.00 34.23 ATOM 2542 CD2 LEU A 330 42.078 44.382 47.285 1.00 34.05 ATOM 2545 CA SAN A 332 33.884 49.37 8.59 51.544 1.00 34.05 ATOM 2545 C GLY A 331 31.8849 37.859 51.544 1.00 35.66 ATOM 2546 C GLY A 331 31.8849 37.859 51.544 1.00 35.61 ATOM 2555 C GAN A 332 36.647 40.951 48.381 1.00 37.01 ATOM 2556 C AN R A 332 36.647 40.951 48.381 1.00 37.01 ATOM 2557 C PRO A 333 33.31.31 40.754 40.275 51.094 1.00 36.54 ATOM 2556 C AN R A 332 36.647 40.951 48.881 1.00 36.54 ATOM 2556 C AN R A 332 36.647 40.951 48.881 1.00 36.54 ATOM 2556 C AN R A 333 33.31.31 40.754 40.260 51.40 1.00 37.47 ATOM 2557 C PRO A 333 33.31.31 40.754 41.984 41.999 41.00 36.554 ATOM 2556 C AN R A 332 33.31.31 40.754 41.984 41.990 41.00 36.554 ATOM 2556 C BN A 333 33.31.31 40.760 41.399 41.399 41.00 36.554 ATOM 2566 C BUN								36.486		1.00 35.91		C
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ATOM 2561 CD PRO A 333 35.180 37.668 48.548 1.00 36.54 ATOM 2562 N GLN A 334 33.743 40.800 48.047 1.00 36.44 ATOM 2563 CA GLN A 334 32.906 41.969 48.130 1.00 36.85 ATOM 2564 C GLN A 334 33.748 43.222 48.057 1.00 36.57 ATOM 2565 O GLN A 334 33.218 44.304 47.868 1.00 36.98 ATOM 2566 CB GLN A 334 31.987 41.940 49.348 1.00 37.31 ATOM 2567 CG GLN A 334 30.685 41.151 49.026 1.00 38.95 ATOM 2568 CD GLN A 334 29.669 41.097 50.171 1.00 40.33 ATOM 2569 OE1 GLN A 334 29.751 41.872 51.137 1.00 41.70 ATOM 2570 NE2 GLN A 334 28.712 40.178 50.061 1.00 39.80 ATOM 2571 N GLU A 335 35.064 43.088 48.159 1.00 35.99												С
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ATOM 2570 NE2 GLN A 334 28.712 40.178 50.061 1.00 39.80 ATOM 2571 N GLU A 335 35.064 43.088 48.159 1.00 35.99				GLN	А	334						C
ATOM 2571 N GLU A 335 35.064 43.088 48.159 1.00 35.99				GLN	A	334						0
ATOM 2572 ON OTT 3 200			N	GLU	Α	335						N N
	MOTA	2572	CA	GLU	A	335						C
												J

ATOM	2573	C	GLU A	335	5	36.229	44.610	46.621	1.00	34.53		С
ATOM										34.20		ō
	2574		GLU A			36.715	45.689	46.338				
MOTA	2575	CB (GLU A	335	5	37.201	44.083	48.894	1.00	35.99		С
MOTA	2576	CG	GLU A	335	5	37.054	44.507	50.354	1.00	37.38		С
	2577											Ċ
ATOM			ĢLU A			38.382	44.592	51.076		40.16		
ATOM	2578	OE1	GLU P	335	5	39.271	45.318	50.570	1.00	42.04		0
MOTA	2579	OE2	GLU A	339	5	38.535	43.952	52.153	1.00	41.52		0
ATOM	2580		VAL A			35.922	43.701	45.706		33.97		N
MOTA	2581	CA	VAL A	7 336	5	36.165	43.901	44.276	1.00	33.49		С
ATOM	2582	C	VAL A	330	6	35.537	45.159	43.670	1.00	33.00		С
MOTA	2583		VAL A			36.194	45.904	42.946		33.01		0
ATOM	2584		VAL A			35.696	42.678	43.473		33.36		С
MOTA	2585	CG1	VAL A	4 33	6	35.726	42.951	41.992	1.00	34.05		С
ATOM	2586	CG2	VAL A	4 33	6	36.582	41.509	43.755	1.00	33.01	•	С
MOTA	2587		GLY 1			34.270	45.406	43.926		32.41		N
ATOM	2588	CA	GLY A	A 33	7	33.675	46.592	43.351	1.00	32.21		С
ATOM	2589	C	GLY A	A 33	7	34.332	47.903	43.724	1.00	31.72		С
	2590		GLY Z					42.859		31.40		0
MOTA						34.682	48.711					
MOTA	2591	N	PRO I	EE A	8	34.433	48.163	45.013	1.00	31.50		И.
ATOM '	2592	CA	PRO I	A 33	8	35.025	49.415	45.470	1.00	31.47		С
MOTA	2593	C	PRO 2			36.387.		44.846		31.60		С
MOTA	2594	O :	PRO 1			36.655	50.756	44.386		31.51		0
MOTA	2595	CB	PRO .	A 33	8	35.065	49.230	46.977	1.00	31.27		С
ATOM	2596	CG	PRO .	A 33	R	33.883	48.376	47.218	1.00	31.08		С
												Č
MOTA	2597	CD	PRO .			33.933	47.359	46.137		31.28		
MOTA	2598	N	LEU	A 33	9	37.219	48.620	44.765	1.00	31.80		N
MOTA	2599	CA	LEU	A 33	9	38.531	48.825	44.182	1.00	32.25		С
ATOM	2600	C	LEU			38.431	49.269	42.740		32.12		C
ATOM	2601	0	LEU	A 33	19	39.130	50.188	42.320	1.00	32.25		0
MOTA	2602	CB	LEU	A 33	19	39.395	47.581	44.278	1.00	32.49		С
MOTA	2603	CG	LEU			40.853	47.920	43.962		33.78		С
ATOM	2604		LEU			41.793	47.121	44.797		34.64		C
ATOM	2605	CD2	LEU	A 33	39	41.146	47.681	42.516	1.00	34.50		С
ATOM	2606	N	LEU	A 34	10	37.567	48.607	41.978	1.00	32.12		N
	2607	CA						40.584		31.85		C
MOTA			LEU			37.385	48.963					
ATOM	2608	С	LEU	A 34	10	36.854	50.376	40.483	1.00	31.56		С
MOTA	2609	0	LEU	A 34	10	37.342	51.169	39.701	1.00	31.42		0
ATOM	2610	СВ	LEU			36.468	47.975	39.888	1 00	31.90		С
												Ċ
ATOM	2611	CG	LEU			37.089	46.598	39.669		32.44		
ATOM	2612	CD1	LEU	A 34	40	36.028	45.636	39.132	1.00	33.11		С
ATOM	2613	CD2	LEU	A 34	40	38.281	46.660	38.728	1.00	31.95		С
ATOM	2614					. 35.865				31.61		N
MOTA	2615	CA	ASN			35.384	52.083			31.82		С
MOTA	2616	С	ASN	A 3	41	36.484	53.109	41.525	1.00	31.45		С
ATOM	2617	0	ASN	A 3	41	36.600	54.119	40.845	1.00	30.80		0
ATOM	2618	СВ	ASN			34.212	52.260	42.177		31.97		Č
MOTA	2619	CG	ASN	A 3	41	32.901	51.883	41.532	1.00	32.77		С
ATOM	2620	OD1	ASN	A 3	41	32.426	52.568	40.614	1.00	34.75		0
MOTA	2621		ASN			32.310	50.789		1 00	31.86		N
MOTA	2622	N		A 3		37.301				31.40		N
ATOM	2623	CA	THR	A 3	42	38.380	53.739	42.880	1.00	31.27		С
MOTA	2624	C		A 3		39.317	53.842			31.14		C
										30.66		
ATOM	2625	0		A 3		39.837						0
MOTA	2626	CB	THR	A 3	42	39.146			1.00	31.43		C
ATOM	2627	OG1	THR	A 3	42	38.448	53.565	45.299	1.00	30.95		0
ATOM	2628		THR			40.500				31.17		C
MOTA	2629			A 3		39.549				31.29		N
MOTA	2630	CA	MET	а з	43	40.406	52.703	39.898	1.00	31.59		С
MOTA	2631	С		A 3		39.970			1.00	31.49		С
	2632											Õ
MOTA				A 3		40.804				31.46		
MOTA	2633	СВ	MET	A 3	43	40.516	51.310	39.314	1.00	31.79		С
	•											

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ATOM	2634	CG	MET	A	343		41.831	50.662	39.629	1.00	32.65		С
	2635	SD	MET				42.271	49.379	38.468		33.09		S
ATOM	2636	CE	MET				41.116	48.304	38.916		34.22		С
ATOM	2637	N	ILE				38.690	53.641	38.418		31.31		N
MOTA	2638	CA	ILE				38.293	54.432	37.265		31.42		С
ATOM	2639	C	ILE				37.708	55.787	37.533		31.14		С
ATOM ATOM	2640	O	ILE				37.752	56.630	36.640		31.01		. 0
ATOM	2641 2642	CB	ILE ILE				37.272	53.708	36.362		31.86		С
ATOM	2643		ILE				35.870	53.866	36.928		33.16		С
ATOM	2644		ILE				37.633 34.876	52.229 53.232	36.118 36.072		32.09		C
ATOM	2645	N			345		37.131	56.050	38.698		35.18 30.88		C
ATOM	2646	CA	LYS				36.455	57.334	38.758		30.88		N
ATOM	2647	C	LYS				37.412	58.468	38.853		30.72		C
ATOM	2648	0	LYS				38.250	58.558	39.743		30.72		0
ATOM	2649	СВ			345		35.315	57.475	39.765		31.14		C
ATOM	2650	CG			345		35.361	56.680	40.977		32.16		c
ATOM	2651	CD			345		33.970	56.273	41.340		33.62		Č
ATOM	2652	CE	LYS	Α	345		33.514	56.873	42.665		34.71		Ċ
ATOM	2653	NZ			345		34.302	56.317	43.840		36.28		N
ATOM	2654	N			346		37.280	59.332	37.870		30.83		N
ATOM	2655	CA			346 .		38.114	.60.504	37.789	1.00	30.66		C
ATOM	2656	С			346		39.345	60.195	37.001	1.00	30.25		С
	2657	0			346		40.147	61.066	36.745		30.00		0
ATOM	2658	N			347		39.454	58.953	36.564		30.42		N
ATOM	2659	CA			347		40.652	58.496	35.923		30.66		С
ATOM	2660	C			347		40.389	57.879	34.566		30.89		С
ATOM	2661	0			347		41.033	58.241	33.588		30.30		0
ATOM ATOM	2662 2663	CB			347		41.350	57.526	36.860		30.88		C
ATOM	2664	CG CD			347 347		41.786	58.177	38.171		30.97		С
ATOM	2665	NE			347		43.129 43.128	57.701	38.636		31.35		С
ATOM	2666	CZ			347		43.128	56.255 55.482	38.597 38.128		30.88		И
ATOM	2667		ARG				45.237	55.962	37.667		29.55 28.44		C
ATOM	2668		ARG				43.876	54.181	38.147		29.95		N N
ATOM	2669	N			348		39.446	56.953	34.480		31.67		N
ATOM	2670	CA			348		39.143	56.377	33.176		32.27	•	C
ATOM	2671	С			348		37.726	56.574	32.689		33.10		č
MOTA	2672	0			348		37.425	56.212	31.557		33.12		ŏ
MOTA	2673	CB	TYR	Α	348		39.422	54.896	33.154		31.96		C
MOTA	2674	CG	TYR	A	348		40.860	54.527	33.253		32.06		C
MOTA	2675		TYR				41.652	54.424	32.114	1.00	31.60		С
ATOM	2676		TYR				41.435	54.256	34.483	1.00	31.75		С
ATOM	2677		TYR				42.980	54.061	32.203	1.00	31.08		C
ATOM	2678		TYR				42.761	53.897	34.580	1.00	32.11		C
ATOM	2679	CZ			348		43.530		33.438		31.05		С
ATOM	2680	ОН			348		44.845	53.427	33.544		29.83	•	0
ATOM	2681	N			349		36.850	57.137	33.507		34.48		N
ATOM ATOM	2682	CA			349 -		35.465	57.275	33.083		35.73		C
ATOM	2683 2684	C			349		35.037	58.643	32.595		36.60		C
ATOM	2685	O			349		35.757	59.640	32.508		37.31		0
ATOM	2686	CB CG			349		34.542	56.900	34.212		35.62		C
ATOM	2687				349 349		34.635	57.864	35.353		37.08		C
ATOM	2688				349		35.398 33.861	58.840	35.308		36.55		0
ATOM	2689				349		33.861	57.604 58.757	36.403 32.276		39.78		N
TER	2690	~			349		22.00T	50.757	26.210	1.00	38.11		0
HETATM		FE			1350		23.364	27.586	28.889	1 00	32.45		ਧਾਹ
HETATM		Cl			1351		22.523	25.412	27.792		37.04		FE C
HETATM		01			1351		23.535	26.092	27.914		39.03		0
HETATM		02			1351		22.557	24.216	27.226		37.33		0
					-					~	555		9

HETATM	2695	C2	AKG Z	A1351	2	21.186	25.964	28.297	1.00				
HETATM	2696	05	AKG A	A1351	2	21.175	27.063	28.807	1.00	33.4	4		
HETATM	2697	C3	AKG A	A1351	1	L9.937	25.139	28.167	1.00	36.1	1		
HETATM	2698	C4	AKG 2	A1351	1	L8.848	25.738	29.055	1.00	36.5	0		
HETATM		C5	AKG 2	A1351		L7.464	25.331	28.632	1.00				
HETATM		03	AKG	A1351	-	L7.276	25.331 24.627 25.771	27.656	1.00				
HETATM		04	AKG :	A1351		16.432	25.771	29.338	1.00				
HETATM		S	SOA	M1352	•	0.300	25.196	43 477	1.00				
		01	504	713E3		1 004	26 117	43.477	1.00	70 5	0		
HETATM		01	504	M1332		1 221	20.117	44.500	1.00	70.5	1		
HETATM		02	504	A1332		1.221	24.413	44.044	1.00	70.5	T.		
HETATM		03	504	A1352		-0.470	24.282	44.306 42.644 44.334 42.633 29.515	1.00	79.5	4		
HETATM		04	SO4	A1352		-0.640	25.951	42.633	1.00	78.0	7		
HETATM	2707	S	SO4	A1353		1.825	28.603	29.515	1.00	77.3	8		
HETATM	2708	01	SO4	A1353		3.041	29.212	30.061	1.00	76.0	5		
HETATM	2709	02	SO4	A1353		2.144	27.528	.28.574	1.00	75.2	4		
HETATM	2710	03	SO4	A1353		1.090	28.086	30.675	1.00	76.5	2		
HETATM	2711	04	SO4	A1353		1.011	29.586	28.783	1.00	76.0	4		
HETATM	2712	S	SO4	A1354		34.403	30.284	38.043	1.00	78.1	.7		
HETATM	2713	01	SO4	A1354.		34.921	31.567	38.516	1.00	75.9	3		
HETATM	2714	02	SO4	A1354		35.240	29.158	38.450	1.00	77.4	12		
HETATM	2715	03 ·	SO4	A1354		33.112	. 30.084	38.686	1.00	75.5	59		
HETATM	2716	04	SO4	A1354		34.303	30.307	36.581	1.00	74.6	50		
НЕТАТМ	2717	0	HOH	7 1		25 824	26.442	29.515 30.061 28.574 30.675 28.783 38.043 38.516 38.450 38.686 36.581 26.175 24.637 25.742	1.00	46.4	13		
UETATU	2712	0	HOH	7 2		27 811	27 709	24 637	1 00	41 3	32		
BETAIN	2710	0	HOH	7 2	•	27.011	30 233	25 7/2	1 00	38 1	18		
CONECT	1/70	2601	поп	4 3		27.307	30.233	23.142	1.00	50			
CONECT	1490	2031											
CONECT	2101	703T	0.00	1470	01.67	1400							
CONECT	2691	2696	2693	3 14/8	2101	1498							
CONECT	2692	2693	2694	4 2695									
				Ţ									
CONECT	2694	2692											
CONECT	2695	2692	269	6 2697									
CONECT	2696	2691	269	5									
CONECT	2697	2695	269	8									
CONECT	2698	2697	269	9									
CONECI	2699	2698	270	0 2701				•					
CONECT	2700	2699	ŀ										
CONECT	2701	2699	ı										
CONECT	2702	2703	270	4 2705	2706								
CONECT	2703	2702											
CONEC	2704	2702	:										
CONECT													
CONECT													
				9 2710	2711								
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CONEC				4 0715	0716								
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CLAIMS

- 1. A method of identifying, screening, characterising or designing a chemical entity which mimics or binds to FIH, which method comprises comparing a structural model of FIH with a structural model for said chemical entity, wherein said structural model of FIH is derived from structural factors or structural coordinates determined by subjecting to X-ray diffraction measurements a crystal comprising FIH.
- 2. Use of the structural co-ordinates obtainable by subjecting a crystal comprising FIH to X-ray diffraction measurements and deducing the structural co-ordinates from the diffraction measurements, to identify, screen, characterise, design or modify a chemical entity.
- 3. A method or use according to claim 1 or 2 in which the structural coordinates are those shown in Table 3.
- 4. A method or use according to any one of the preceding claims, wherein said chemical entity binds to FIH.
 - 5. A method or use according to any one of the preceding claims, wherein said chemical entity is selected to inhibit the asparaginyl hydroxylase activity of FIH.
- 6. A method or use according to any one of the preceding claims further comprising contacting said chemical entity with HIF or a fragment thereof or a homologue of either thereof incorporating asparagine 803 with FIH or a homologue thereof which maintains the asparaginyl hydroxylase activity of FIH and monitoring for hydroxylation of asparagine 803.
 - 7. A chemical entity identified by a method for use according to any one of the preceding claims, wherein said chemical entity inhibits the asparaginyl hydroxylase activity of FIH.
 - 8. A chemical entity according to claim 7 wherein said chemical entity inhibits hydroxylation of the asparagine position 803 of HIF by FIH.
- 9. A chemical entity according to claim 7 wherein said chemical entity inhibits dimerisation of FIH.

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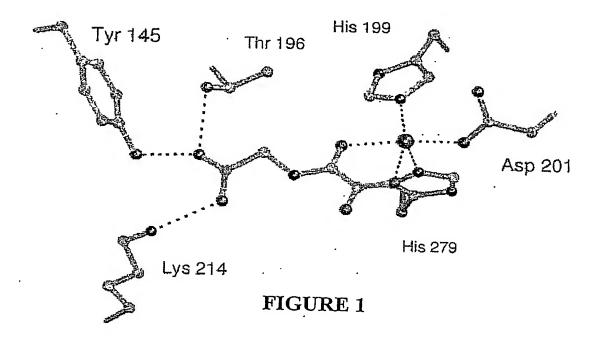
- 10. A chemical entity according to claim 9 wherein said chemical entity binds to residues that form the dimerisation interface of FIH, selected from residues 330 to 346 of FIH.
- 11. A chemical entity according to claim 7 wherein said chemical entity binds to iron, or prevents Fe(II) binding to FIH.

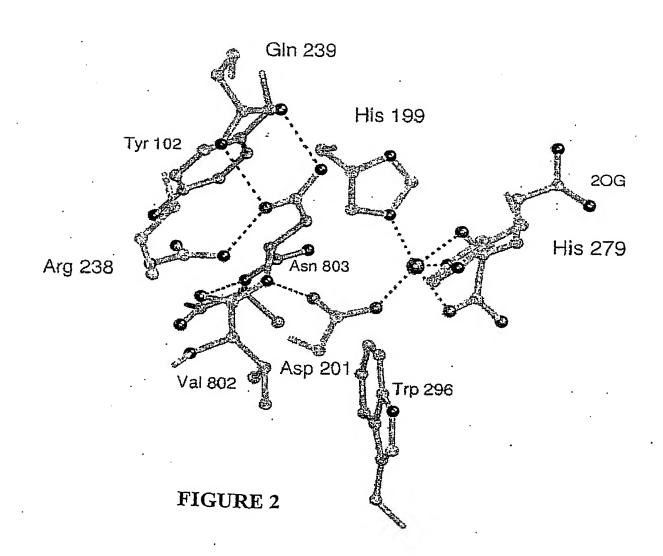
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- 12. A chemical entity according to claim 7 wherein said chemical entity disrupts 2-oxoglutarate binding to FIH.
- 13. A chemical entity according to claim 12 wherein said chemical entity interferes with the interactions at residues 214, 196 and 145 of FIH, or which interrupts the interactions of 20G with residues 281, 186, 188, 207 or 196 of FIH.
- 14. A chemical entity according to claim 7 wherein said chemical entity interrupts binding of FIH for Asn 803 of HIF, preferably, by interfering with binding of HIF at residues 102, 239 or 238 of HIF.
- 15. A chemical entity according to claim 7 which interferes with Site 1 binding of CAD of HIF to FIH and which exploits electrostatic, hydrogen binding and/or hydrophobic interactions with one or more residues selected from 102, 104, 106, 201, 202, 147, 239, 299-303, 313, 317, 318, 321, 324, 238, 296 or 321 to 324 of FIH.
- 16. A chemical entity according to claim 14 wherein said chemical entity interferes with binding of CAD of HIF to FIH at Site 2, and exploits electrostatic, hydrogen binding and/or hydrophobic interactions with residues 149, 150, 151, 152, 159, 162, 163, 167, 181, 182, 183, 184 or 185.
 - 17. A chemical entity according any of one of claims 7 to 16 for use in a method of treatment.
- 25 18. A chemical entity according to claim 17 for use in the treatment of ischaemia and/or to promote antiogenesis.





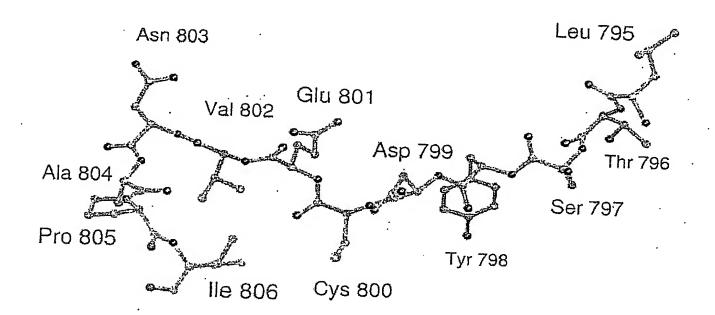


FIGURE 3

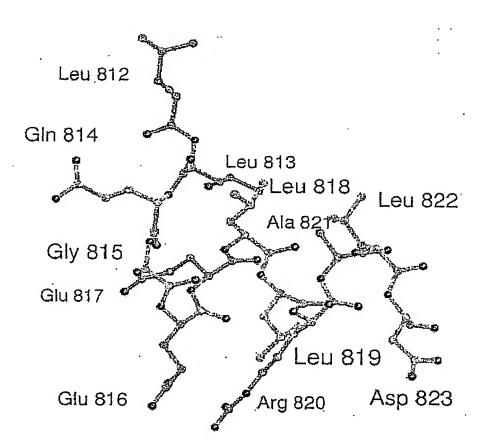


FIGURE 4

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